Annual Report 2021

Jožef Stefan Institute, Ljubljana, Slovenia

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INTRODUCTION

Another year marked by the Covid-19 health crisis is behind us. A period during which our researchers also had to learn the skills of crisis management. Above all, we continued to try our best to help society adapt to the new conditions, while we have had to come to terms with the fact that, even after overcoming all the problems, the "new normal" will be different from the old one, and this includes the role played by science. If, in previous years we only aimed to learn about the new and the

unknown, in the future we will have to use existing knowledge much more effectively. The Covid-19 vaccine is a good example of humanity mastering a certain technology, but then it has to face a problem of sufficient magnitude before deciding to implement it.

At the JSI we quickly adapted to a different way of working. Home working became routine, and we made greater use of modern technologies so that we can operate in this way. We also learned about their strengths and weaknesses. While we have been as successful in terms of publishing the results of our research as in the non-crisis years, the experimental work has suffered considerably. Despite the high level of digitization, these activities are still based on the work of human hands. In the future, research has a lot of work to do, but with the help of robotization and the use of artificial intelligence, it will bring the work in laboratories up to the level that we already achieve today in the automation of business processes and manufacturing.

From left: Director Prof. Boštjan Zalar and Dr. Josef Aschbacher, Director General of the European Space Agency (ESA) signed the loan agreement for the Human Centrifuge in Planica.
In the second row: Simon Zajc, State Secretary, Ministry for Economic Development and Technology; Dr. Franci Petek, Director of Institute of Sports of the Republic of Slovenia, Planica; and Dr. Simona Kustec, Minister of Education, Science and Sport

At the end of 2021, Slovenian research finally saw new legislation governing the field of research, development and innovation. This gives public research institutes greater autonomy in their research work. The JSI has become the owner of all its real estate, and it can now decide for itself about how to distribute the funds allocated by the state for stable financing between research programmes and different economic needs. Above all, we are looking forward to the fact that the funds for our activities will increase significantly in the coming years. We are not worried that we will not be able to absorb the growth, if only the country would come up with some much-needed support, such as improving the conditions for implementing human-resources policy and greater internationalisation by reducing the administrative obstacles to the recruitment of researchers from abroad.

I am particularly pleased to note that in 2021, at the JSI we again increased the number of publications in international journals. According to the data in the Web of Science database, we were cited almost 53,000 times. JSI researchers were awarded 22 doctorates, 21 patents, and 14 scientific and professional monographs were published. In addition, we attracted 38 new young researchers. From a total of 1089 projects, 302 were international, including 4 projects from the European Research Council. Our 1126 employees generated more than €62 M in revenue, of which more than €6 M was earned on the national and more than €10.5 M on the international market.

Prof. Boštjan Zalar
Director of the Jožef Stefan Institute

A BRIEF HISTORY OF THE JOŽEF STEFAN INSTITUTE

1946

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

1949

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

1952

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

1954

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

1956

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

1958

~ Institute reorganised and new fields of activity defined: nuclear physics, solid-state physics, chemistry, and radiobiology

1959

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

Mass spectrometer at the JSI (about 1960)

1962

~ One of the first compounds of a noble gas, XeF_6, synthesised at the institute

~ The first computer for research, ZUSE Z23, installed

1966

~ Nuclear research reactor TRIGA starts operation

1968

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

1969

~ Institute is renamed as the Jožef Stefan Institute

1970

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

1971

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

Institute buildings after the opening in 1953

1972

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

1974

~ Collaboration with the international centre CERN in the field of high-energy physics started

~ SEPO group for evaluating environmental interventions is established

1976

~ First Yugoslav 8-bit processor computer DARTA 80

1979

~ Contract defining cooperation between the Jožef Stefan Institute and the Nuclear Power Plant Krško is signed

~ First robot in Slovenia is constructed

1982

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

1983

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

The Reactor Centre, Podgorica, built in 1966

1985

~ "2000 New Young Researchers" project established by the Slovenian Research Council

~ Centre for Hard Coatings established by the Jožef Stefan Institute and the firm SMELT

The beginnings of robotics at the JSI, in 1985

1987

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

1989

~ Milan Čopič Nuclear Training Centre established

1990

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

1992

~ New technology centres established by the Ministry of Science and Technology

~ Jožef Stefan Institute restructured by the Slovenian Government as a public research institution

~ Jožef Stefan Technology Park founded, later to become the Ljubljana Technology Park

1995

~ Jožef Stefan Institute is a co-founder of the international postgraduate school for environmental sciences, the Nova Gorica Polytechnic

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

1997

~ 3.5-MeV electrostatic accelerator, TANDETRON, installed

1999

~ Jožef Stefan Institute celebrates its 50th anniversary

2004

~ Jožef Stefan International Postgraduate School established

~ 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

2013

~ First ERC Grant awarded to researcher at JSI

2015

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

2020

~ International Research Centre for Artificial Intelligence was established under the auspices of UNESCO

~ Center for Technology Transfer and Innovation spearheaded Innovation Fund initiative resulting in funding for six successful JSI research projects to increase the technology TRL

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

FORMER DIRECTORS

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

Prof. Anton Peterlin, Founder and first Director of the Jožef Stefan Institute, 1949–1955

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Prof. Danilo Zavrtanik, 1992–1996

Prof. Vito Turk, 1996–2005

Prof. Jadran Lenarčič, 2005–2020

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Reactor Engineering (R-4)
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[1] until 30 November 2021   [2] since 1 December 2021

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University of Nova Gorica

Jožef Stefan International Postgraduate School

Technology Centres

Nanotesla Institute Ljubljana

Development Centre for Hydrogen Technologies

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

Centres of Excellence

Nanocenter - Center of Excellence in Nanoscience and Nanotechnology

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

Centre of Excellence NAMASTE

Centre of Excellence for Polymer Materials and Technologies (PoliMaT)

EN-FIST Centre of Excellence

CEBIC Centre of Excellence for Biosensors, Instrumentation and Process Control

CO NOT: Centre of Excellence for Low-Carbon Technologies

Centre of Excellence for Space Sciences and Technologies SPACE-SI

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Assistant Director for EU Affairs
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Prof. Igor Muševič, *Deputy President since 20. 05. 2021*
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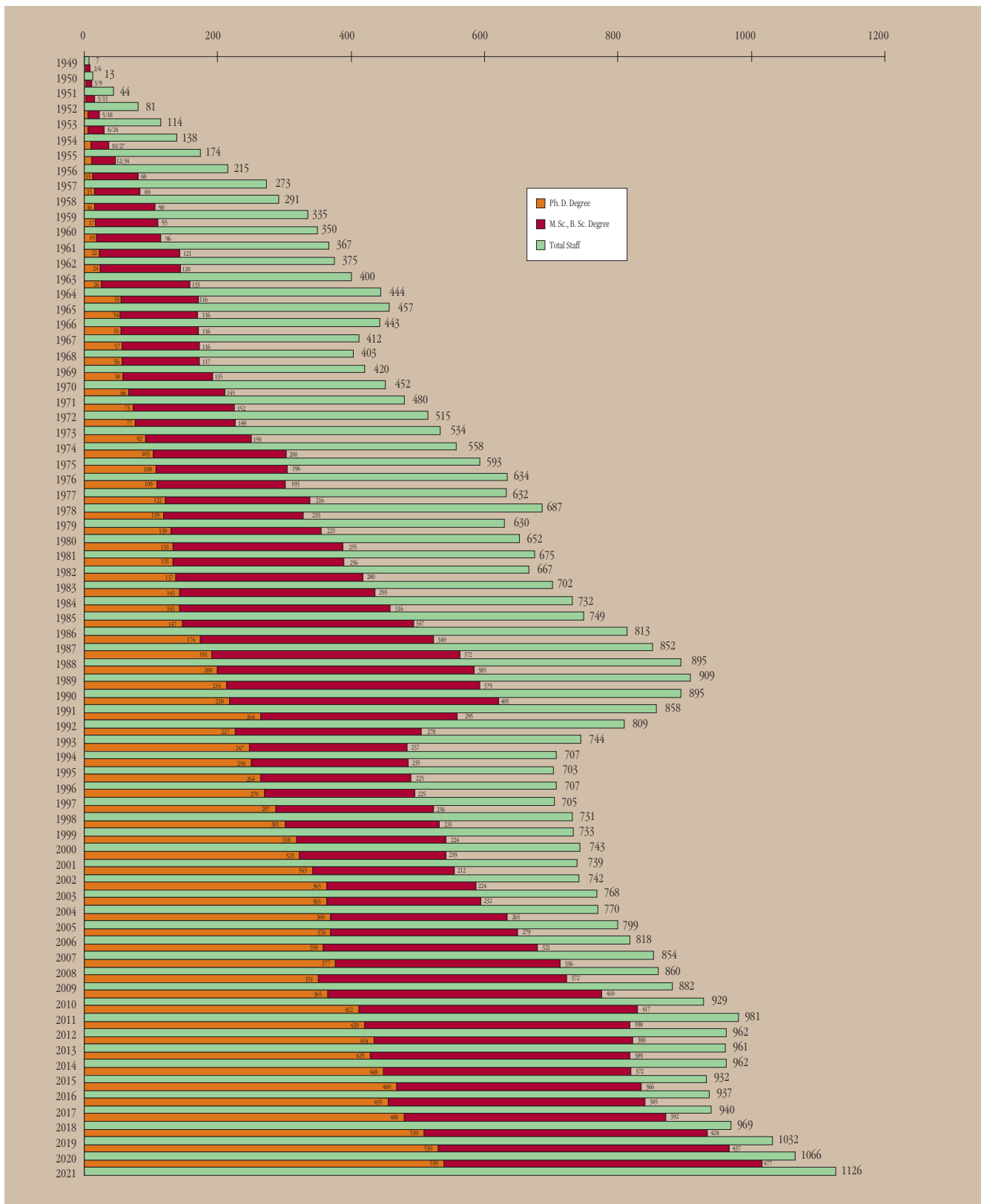Prof. John Ryan, University of Oxford, Oxford, United Kingdom
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1949-2021

Legend:
- Ph. D. Degree
- M. Sc., B. Sc. Degree
- Total Staff

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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

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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)

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

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Prof. Andrej Župančič✝, Slovenian Academy of Sciences and Arts, Ljubljana, Slovenia

INTERNATIONAL COOPERATION

Multilateral international cooperation	No. of projects
HORIZON EUROPE (OE, EDF, EIT) and HORIZON EUROPE - EURATOM	2
H2020 (EUROPEAN INSTITUTE OF INNOVATION AND TECHNOLOGY, EXCELLENT SCIENCE, EURATOM, INDUSTRIAL LEADERSHIP, SOCIETAL CHALLENGES, SPREADING EXCELLENCE AND WIDENING PARTICIPATION, SCIENCE WITH AND FOR SOCIETY) and H2020 - EURATOM	120
ESRR (INTERREG, MED, CEP, KC, SRIP, SPS, KKP, RZ, RI-SI, RR...)	19
OTHER EU PROJECTS (COST, IAEA, ICTP, JRC, ESA, CEF, EMPIR, ERASMUS+, LIFE+,...)	104
OTHER PROJECTS (CERN, KEK, CEA, EURAC, WHO...)	106
TOTAL	**351**

Bilateral cooperation	No. of projects
Austria	4
Bosnia and Herzegovina	1
Denmark	2
Germany	8
France	6
Croatia	6
Italy	3
Japan	4

Bilateral cooperation	No. of projects
Latvia	1
Montenegro	2
Norway	1
Russia	1
Serbia	5
Turkey	2
USA	35
TOTAL	**81**

ERC PROJECTS

1. H2020 - Cell-Lasers; Intracellular Lasers: Coupling of Optical Resonances with Biological Processes
   Asst. Prof. Matjaž Humar (F-5)

2. H2020 - LOGOS; Light-Operated Logic Circuits from Photonic Soft-Matter
   Prof. Igor Muševič (F-5)

3. H2020 - FAIME; Flavour Anomalies with advanced particle Identification MEthods
   Prof. Peter Križan (F-9)

4. H2020 - HiPeR-F; Challenging the Oxidation-State Limitations of the Periodic Table via High-Pressure Fluorine Chemistry
   Asst. Prof. Matic Lozinšek (K-1)

erc
European Research Council
Established by the European Commission

COOPERATION WITH HIGHER-EDUCATION ESTABLISHMENTS

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49. **Prof. Primož Ziherl**, University of Ljubljana, Faculty of Mathematics and Physics
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Assistants and researchers

1. **Dr. Jurij Leskovec**, Stanford University, Palo Alto, California, USA
2. **Dr. Jure Pražnikar**, University of Primorska, Faculty of Mathematics, Natural Sciences and Information Technologies, Koper
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142. **Prof. Kristina Žužek Rožman**, IPS, Ljubljana

Assistants and researchers

1. **Dr. Tilen Brecelj**, University of Ljubljana, Faculty of Mathematics and Physics
2. **Dr. Martin Draksler**, University of Ljubljana, Faculty of Mathematics and Physics
3. **Dr. Tome Eftimov**, University of Ljubljana, Faculty of Computer and Information Science
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REVENUES JSI (€) AND NUMBER OF PROJECTS

	2021	Contribution 2021	2020	Contribution 2020	Index 2021/2020	No. of Projects in 2021
National Agencies and Ministries	44,596,210	71.4 %	41,157,432	72.7 %	108.4	472
National Market	6,896,083	11.0 %	6,081,337	10.7 %	113.4	315
International Market	10,648,758	17.1 %	9,235,685	16.3 %	115.3	302
Other Revenues	309,334	0.5 %	124,806	0.2 %	247.9	
TOTAL	**62,450,385**	**100.0 %**	**56,599,260**	**100.0 %**	**110.3**	**1089**

Revenues 2020/2021 (€M))
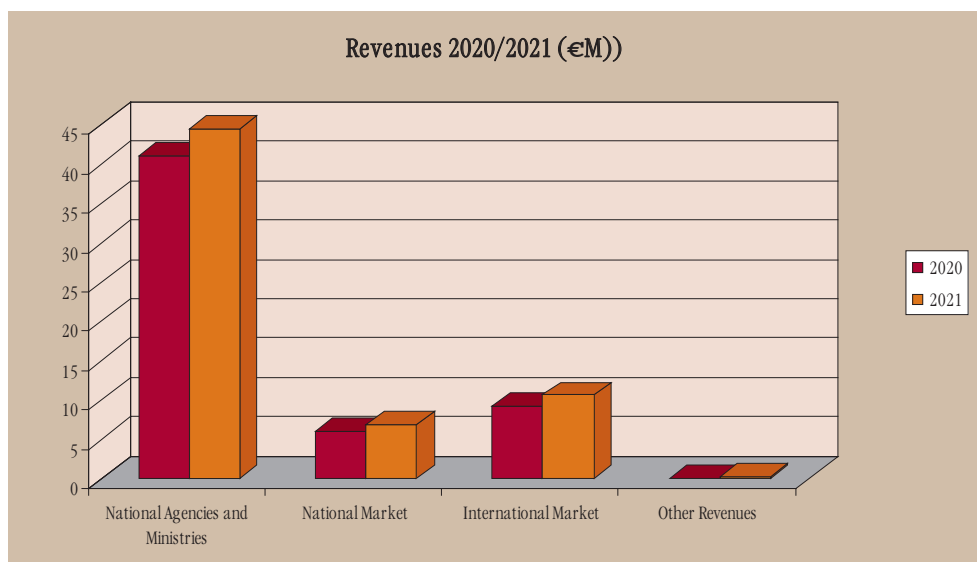
POSTGRADUATES FINANCED 1985-2021

by Slovenian Research Agency
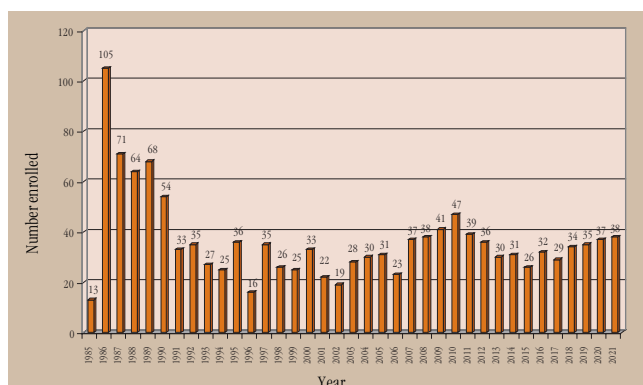
by Industry

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1977-2021

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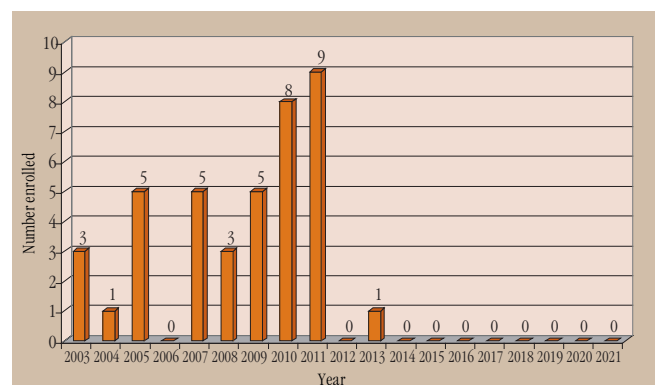| Year	FMF		FKKT UNI LJ	FKKT UNI MB	NTF	FDV	FA	BF	FE and FRI	Other UNI LJ	FG and FERI	UNG	IPS	Total
	Physics	Mathematics												
... 1989	242	75	144					4	181	21	4			671
1990	26	5	11					2	25		1			70
1991	23	2	9					2	24	2	1			63
1992	22	3	16					3	17	1				62
1993	21	1	15					3	13	1				54
1994	7	1	8					3	6					25
1995	2		9					3	5					19
1996	2		9					3	5					19
1997	2		12					1	4		1			20
1998	1		6					1	7		1			16
1999	2		7					4	7					20
2000	1		5					3	9					18
2001	3		13					3	10					29
2002	4		20					3	10					37
2003	3		18					2	12	1				36
2004	4		17					1	15	1	2	2		42
2005	3		12			1		2	19		2	1		40
2006	2		12			1		1	17		2	2		37
2007	3		14			1		2	18		2	1		41
2008	2	1	13	3		1		2	15		1	1		39
2009	2	1	17	4		1		5	16		1	2		49
2010	2		11	5	2	1	1	3	10		1	2	5	43
2011	2	1	11	5	4	1	1	4	7		1		6	43
2012	2		10	6	3	1		3	6				5	36
2013	3	2	3	2	1		1		2	2			6	22
2014	14	6	3		2		1		3	2			1	32
2015	21	6	4		1				9	1			10	52
2016	16	2	5						7	1			15	46
2017	11	2	4					2	7				12	38
2018	9	3	5					2	6	1	1		7	34
2019	16	1	5						7		1		12	42
2020	17	1	4						5	1			8	36
2021	19		3						5	1			6	34
TOTAL	509	113	455	25	13	8	4	67	509	36	22	11	93	1865

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FDV	Faculty of Social Sciences, University of Ljubljana
FA	Faculty of Administration, University of Ljubljana
BF	Biotechnical Faculty, University of Ljubljana
FE	Faculty of Electrical Engineering, University of Ljubljana
FRI	Faculty of Computer and Information Science, University of Ljubljana
FG	Faculty of Civil Engineering, University of Maribor
FERI	Faculty of Electrical Engineering and Computer Science, University of Maribor
UNG	University of Nova Gorica
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PATENTS GRANTED

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14. Vid Bobnar, Barbara Malič, Aleksander Matavž, A method for producing polymeric surface modification layers, SI25887 (A), Slovenian Intellectual Property Office, 31. 03. 2021.

ART EXHIBITIONS AT THE JSI

Barbara Kastelec, 18. January–15. Februar

Ivo Mršnik, 15. Februar–15. March

Tone in France Kralj, 15. March–12. April

Milena Gregorčič, 12. April–10. May

Arjan Pregl, 10. May–7. June

Melita Vovk, 7. June –5. July

Vojko Gašperut – Gašper, 5. July–2. August

Jean Duncan, 2. August–6. September

Polona Petek, 6. September–4. October

Marta Bartolj, 4. October–8. November

Darko Slavec, 8. November–6. December

Saša Bezjak, 6. December–10. January 2022

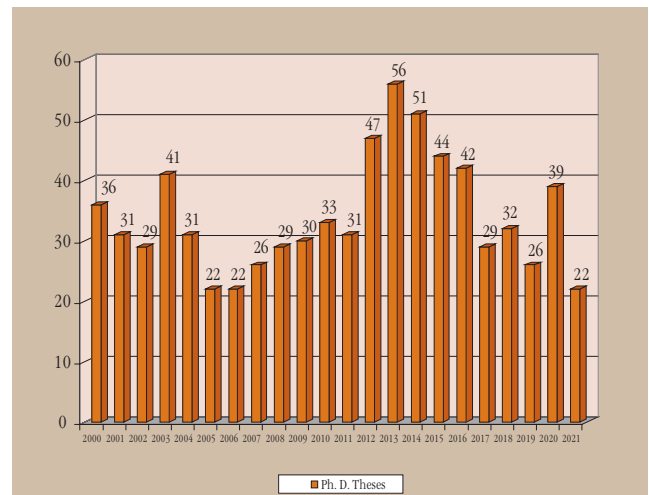Barbara Kastelec at the opening of her exhibition

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Department	Original Articles*	Books	Patent Appl. and Grants	Ph. D. Theses
Department of Theoretical Physics (F-1)	85	1		2
Department of Low and Medium Energy Physics (F-2)	60	2		2
Department of Thin Films and Surfaces (F-3)	13			
Department of Surface Engineering and Optoelectronics (F-4)	67		3	
Department of Solid State Physics (F-5)	173	2	4	3
Department of Gaseous Electronics (F-6)	50		1	
Department for Complex Matter (F-7)	50		1	1
Department of Reactor Physics (F-8)	73			1
Department of Experimental Particle Physics (F-9)	109			
Department of Inorganic Chemistry and Technology (K-1)	30			
Department of Physical and Organic Chemistry (K-3)	27			
Electronic Ceramics Department (K-5)	59		1	
Department for Nanostructured Materials (K-7)	71		4	3
Department for Synthesis of Materials (K-8)	22		1	
Department for Advanced Materials (K-9)	52			1
Department of Biochemistry, Molecular and Structural Biology (B-1)	23		3	
Department of Molecular and Biomedical sciences (B-2)	14			
Department of Biotechnology (B-3)	32		1	1
Department of Environmental Sciences (O-2)	94		2	2
Department of Automation, Biocybernetics and Robotics (E-1)	70		3	1
Department of Systems and Control (E-2)	38	1		1
Artificial Intelligence Laboratory (E-3)	55			1
Laboratory for Open Systems and Networks (E-5)	20			1
Department of Communication Systems (E-6)	61			1
Computer Systems Department (E-7)	57	1		
Department of Knowledge Technologies (E-8)	131	2		
Department of Intelligent Systems (E-9)	65	1	1	
Department of Reactor Engineering (R-4)	40			1
Reactor Infrastructure Centre (RIC)	10			
Science Information Centre (SIC)	1			
Energy Efficiency Centre (EEC)	10	3		
Centre for Electron Microscopy and Microanalysis (CEMM)	6			
Centre for Knowledge Transfer in Information Technologies (CT-3)	2			
Radiation Protection Unit (SVPIS)	1	1		
Centre for Technology Transfer and Innovation (CTT)	22	1		
Centre Factories of the Future (CFOF)	2			
Jožef Stefan Institute	1523	14	21	22

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

COMPLETED THESES UNTIL 2021

Year	Ph. D. Theses
...2000	560
2001	31
2002	29
2003	41
2004	31
2005	22
2006	22
2007	26
2008	29
2009	30
2010	33

Year	Ph. D. Theses
2011	31
2012	47
2013	56
2014	51
2015	44
2016	42
2017	29
2018	32
2019	26
2020	39
2021	22
TOTAL	1273

AWARDS AND APPOINTMENTS

AWARDS MADE TO JSI RESEARCHERS BY THE REPUBLIC OF SLOVENIA

Zois and Puh Awards and Zois Certificate of Recognition

Goran Dražić
Presented with the Zois Award for for top achievements in the field of transmission electron microscopy of materials

Matej Kanduč
Presented with the Zois Certificate of Recognition for significant scientific achievements in hydration and thermoresponsive hydrogel research

Nataša Vaupotič
Presented with the Zois Certificate of Recognition for research in the field of modelling of structures and resonant response of multidimensional thermotropic phases

Borka Jerman Blažič
Presented with the Puh Award for achievements in the field of information and communication technologies

Luka Drinovec, Griša Močnik, R&D departments of Aerosol, d. o. o. and Robomed, d. o. o. Presented with the Puh Award for outstanding achievements in the development of methods for measuring aerosol absorption

Award in the Field of Education

Samo Kralj
Award for outstanding achievements in higher education, Committee for awarding prizes for education in the Republic of Slovenia

The winners of Zois anf Puh Awards and Zois Certificate of Recognition: Prof. Goran Dražić, Prof. Griša Močnik, Dr. Luka Drinovec, Prof. Borka Jerman Blažič, Prof. Nataša Vaupotič and Dr. Matej Kanduč

JSI AWARDS AND APPOINTMENTS

Blinc Award

Martin Čopič

Blinc Award for lifetime achievement in physics

Uroš Tkalec

Blinc Award for a research in the field of imbalanced complex fluids that was published in Nature Communications

Miha Ravnik

Blinc Award for physicist at the beginning of their career

The Jožef Stefan Golden Emblem Prize

presented to the following for doctoral theses with high impact :

Sara Drvarič Talian

Study of selected processes and parameters influencing the internal resistance in lithium-sulfur batteries

Špela Zupančič

Development of core-shell nanofibers for innovative periodontal disease treatment

Martin Gjoreski

A fusion of classical and deep machine learning for mobile health and behavior monitoring with wearable sensors

The Blinc award is conferred by the Jožef Stefan Institute and the Faculty of Mathematics and Physics, University of Ljubljana. The winners of the Blinc awards (from left): Prof. Miha Ravnik, Prof. Martin Čopič and Asst. Prof. Uroš Tkalec.

OTHER SELECTED AWARDS TO JSI RESEARCHERS

Danfoss Trata and Department of Systems and Control at the JSI are the recipients of the TARAS award for 2021 for the development of intelligent motor drives, which is presented by the IRT Industrial Forum, the organiser of the main professional event for Slovenian industry, to recognise the most successful cooperation between business and the research and development environment in the field of innovation, development and technology, Portorož, Slovenija

Members of the Department of Reactor Physics, Award of the Slovenian Research Agency (ARRS) for Research Activity of the Republic of Slovenia 'Excellent in Science 2021' in the category Technology, subcategory Energy for the work "Sterilization of polypropylene membranes of facepiece respirators by ionizing radiation"

Members of the Department of Intelligent Systems: Award for current work in the area of the information society; Ljubljana, Slovenia; Programme and Organising Committee of the Information Society 2021 multiconference; second place at the XPrize Pandemic Response Challenge

Team JSI vs COVID: Matej Cigale, Carlo De Masi, Erik Dovgan, Matjaž Gams, Anton Gradišek, Vito Janko, Mitja Luštrek, Matej Marinko, Nina Reščič, David Susič, Tea Tušar, Aljoša Vodopija, Second place at the XPrize Pandemic Response Challenge; virtual; XPrize Foundation, Culver City, California, USA; methods for predicting COVID-19 infections and recommending countermeasures

Andreja Benčan Golob, Goran Dražić, Barbara Malič, Mojca Otoničar, Tadej Rojac, Hana Uršič Nemevšek, Achievement for the paper "Connecting the Multiscale Structure with Macroscopic Response of Relaxor Ferroelectrics" was included in the selection Excellent in Science ARRS 2021

Monika Biasizzo, Young Investigator Award Nomination: Best Speaker at 38th Winter School on proteinases and their inhibitors, ASBMB virtual conference, Impaired autophagy and increased susceptibility to LPS-induced sepsis in cystatin C-deficient mice.

Tilen Brecelj and Tadej Petrič, Best Research Paper Award, Futuroscope-Poitiers, France, RAAD 2021, Angular Dependency of the Zero Moment Point

Oana-Andreea Condurache, Winner of the 3rd place at Virtual Workshop Contest: YCN Pitch me your Idea!, Young Ceramicist Network Pitch Contest

Oana-Andreea Condurache, Winner of the 3rd place at the Student Paper Contest, 27th Annual Meeting the Slovenian Chemical Society (SKD 2021)

Uroš Cvelbar, Martina Modic, et al., Golden Award for Innovation of the Chamber of Commerce of Dolenjska and Bela Krajina 2021.

Alja Čontala, 13th Jožef Stefan IPSS Conference and 15th CMBE Day, Greenest Research Award

Matjaž Dlouhy, First prize in the category best student lecture entitled "The effect of corrosion relevant species on the adsorption of imidazole on copper", at the 27th annual meeting of the Slovenian Chemical Society entitled "Slovenian Chemical Days 2020", September 22–24, 2021.

Carola Doerr, Tome Eftimov and Anja Janković, Best Paper Award at EvoApps 2021 as part of EvoStar: EvoApplications: Towards Feature-Based Performance Regression/ Using Trajectory Data

Sabina Drofenik, Krka recognition 2021, Novo mesto, Krka, pharmaceutical company. Research project: Description of the mechanism and interdependence of the action of two nosehorned viper venom proteins, secretory phospholipase A_2 and chymotrypsin inhibitor (co-mentor Prof. Igor Križaj).

Tome Eftimov, Dragi Kocev, Gorjan Popovski, Matej Petković in Barbara Koroušić Seljak, ARRS Award Excellent in Science 2021. They received the award in the field of interdisciplinary research with the title of the article: The impact of the COVID-19 pandemic on eating habits.

Tomaž Erjavec, Steven Krauwer Award of the CLARIN research infrastructure for his work on the compilation of the multilingual ParlaMint corpus of parliamentary debates

Matjaž Gams, Urša Klun, Primož Kocuvan, Tine Kolenik, Best paper award of the Insieme project Workshop, Programme and organization committee of the Insieme

project Workshop, International multiconference Information Society, IS2021, "Intelligent cognitive assistant technology for (mental) health in the ISE-EMH project"

Matjaž Gams, David Susič, Janez Tomšič, Award for best workshop paper of the project Insieme, Ljubljana, Programme and Organizing Committee of the Project Insieme Workshop, International Multiconference Information Society, IS2021, Effectiveness of non-pharmaceutical interventions in handling the COVID-19 pandemic: Review of related studies"

Timotej Gašpar, Vodovnik award for doctoral studies, Ljubljana, Faculty of Electrical Engineering, University of Ljubljana, Technologies for fast reconfiguration of adaptive robotic workcells

Anton Gradišek, Award for the best oral presentation at Ecobalt 2021 with the title "Particle Removal Efficiency of Face Masks During the Covid-19 Pandemic", Riga, Latvia (virtual)

Ester Heath and David Škufca, Recognition for the best research achievement of the University of Ljubljana in 2021. University of Ljubljana, Ljubljana, Slovenia. Modern organic pollutants - how can we control them with algae?

Nataša Hojnik, Award of Slovenian Research Agency – Excellent in Science 2021, Unravelling the pathways of air plasma induced aflatoxin B1 degradation and detoxification.

Adrijan Ivanušec, Jernej Šribar, **Peter Veranič**, Maja Zorovič, **Marko Živin and Igor Križaj**, Best Poster Award: 8th Oxford Venoms and Toxins Meeting (virtual), Work title: Mammalian secreted phospholipase A2 group IIA binds to the same mitochondrial receptor as its β-neurotoxic orthologue from snake venom

Ita Junkar, Metka Benčina, Matic Resnik, Rok Zaplotnik, Best innovation with commercial potential award, Center for Technology Transfer and Innovation at the Jožef Stefan Institute, Novel surface finishing procedures for medical devices, especially vascular stents.

Aljaž Kavčič, The Prešeren Award for his master's thesis "Microscopy and sensing through scattering tissues using optical microresonators" (mentor Asst. Prof. Matjaž Humar), Ljubljana, University of Ljubljana

Adem Kikaj and Mako Bohanec, best student paper award at the conference ICDSST 2021 (7th International Conference on Decision Support System Technology, Loughborough, UK) for their paper titled "DEX2Web - a web-based software implementing the multiple-criteria decision-making method DEX".

Dragi Kocev, Article "COVID-19 pandemic changes the food consumption patterns" was among 21 selected achievements in the field of interdisciplinary research by the Slovenian Research Agency.

Janez Kokalj, Matjaž Leskovar, Mitja Uršič, Best Technical Track Paper (ENYGF Conference, Tarragona, Spain) Jóvenes Nucleares, Sociedad Nuclear Española and ENS YGN, "Model for premixed layer formation in stratified fuel-coolant configuration and its application"

Boško Koloski in Bojan Evkoski, Prize for winning the GreenHack Hecaton

Mihael Boštjan Končar, Matej Tekavčič, Mitja Uršič, Young Author Award (International Conference Nuclear Energy for New Europe 2021, Portorož, Slovenia) Nuclear Society of Slovenia, "Film boiling simulation around cylinder with ANSYS Fluent"

Tina Kosjek, Excellent Reviewer Award 2021, Journal of Hazardous Materials, Elsevier

Jan Kren, Best Paper by a Young Researcher Award (Symposium on Advances in Computational Heat Transfer-21, virtual) International Centre for Heat and Mass Transfer, "Numerical analysis of turbulent heat transfer in rectangular duct"

Danjela Kuščer, Silver Award for Innovation: "Manufacture of transparent electrodes from solutions of affordable conductive oxides using screen printing" awarded by Chamber of Comerce Zasavje

Matic Lozinšek, achievement "The first compounds that simultaneously contain krypton and xenon" was included in the Excellent in Science selection 2021, ARRS

Carlo De Masi, Simon Stankoski, Vincent Cergolj, Mitja Luštrek, Best paper award at Slovenian Conference on Artificial Intelligence 2021; Ljubljana, Slovenia; Programme committee of the Slovenian Conference on Artificial Intelligence 2021; paper Intent recognition and drinking detection for assisting kitchen-based activities

Anže Mraz, Winner of the "Fernando Tommasini" award for the most comprehensible talk at the COROSSANO 2021 workshop

Aleš Mrzel and Damjan Vengust, Winners of bronze medal of ARCA 2021 award: Method for the synthesis of metal molybdates and tungstates from molybdenum and tungsten carbides and nitrides; National and University Library in Zagreb, Croatia, 14–16 October 2021

Sebastjan Nemec was awarded the 2nd place in the Best student presentation competition on the SCS Annual Meeting 2021 conference in Portorož (22.–24.9.2021)

Helena Plešnik, Krka's recognition for a master's thesis. Novo mesto, Krka d. d. Determination of bacterial lignin degradation products by liquid chromatography coupled to mass spectrometry

Kity Požek, Adrijana Leonardi, Milan Kojić and Igor Križaj, Best Poster Award: 8th Oxford Venoms and Toxins Meeting (virtual), Work title: Production and characterization of recombinant VaaMPIII-3, a disintegrin like/cysteine rich protein from Vipera a. ammodytes venom.

Kity Požek, Besst essay competition: Hamish Ogston Foundation, London, United Kingdom, Work title: The impact of the Covid-19 pandemic on snakebite research and treatment.

Nina Reščič, Vito Janko, David Susič, Carlo De Masi, Aljoša Vodopija, Matej Marinko, Tea Tušar, Erik Dovgan, Matej Cigale, Anton Gradišek, Matjaž Gams, Mitja Luštrek, Best paper award at the ETAI 2021 conference; virtual / Skopje, North Macedonia; paper Finding efficient intervention plans against COVID-19

Jerica Sabotič, 3rd place in the University of Ljubljana Rector's Award for the best innovation in 2021, Ljubljana, University of Ljubljana Rector Prof. Gregor Majdič, SIMBA – Simultaneous detection of antimicrobial and antibiofilm activities.

Andrej Seljak, Rok Dolenec, Rok Pestotnik, Peter Križan, Samo Korpar, Best innovative projects within public research organizations for the economy in 2021 prize Title: Real-time fluorescence lifetime acquisition system – RfLAS, Center for Technology Transfer and Innovation, Jožef Stefan Institute, Ljubljana, Slovenia

Emanuela Senjor, Dean's Award, Ljubljana, Slovenia, University of Ljubljana, Faculty of Pharmacy, for the paper Cystatin F acts as a mediator of immune suppression in glioblastoma published in Cellular oncology.

Matjaž Spreitzer, Srečo Škapin, Silver award of the CCIS for the innovation Green Energy from aluminium waste, Maribor, Chamber of Commerce and Industry of Slovenia.

Matej Šadl, "Alessandro de Vita" award for curiosity and multidisciplinary approach at Crossnano Crossborder Workshop in Nanoscience and Nanotechnology 2021

Matej Šadl, Winner of the 2nd place at student competition "2021 Joint ISAF ISIF-PMF virtual conference"

Sašo Šturm, Kristina Žužek, Xuan Xu, Silver Medal for Innovation at the ARCA International Exhibition "Environmentally friendly and energy efficient method for recovery of rare earth elements", awarded by the Croatian Association of Innovators, Zagreb, Croatia.

Žiga Tkalec, Award for the best poster at the Jožef Stefan International Postgraduate School Conference and KMBO Conference, Ljubljana, Jožef Stefan International Postgraduate School. Unexpected exposure of children: novel non-targeted screening workflow

Tomaž Tomše, a scholarship recipient for research and for a new approach towards the manufacture of advanced multicomponent Nd-Fe-B permanent magnets for electromotors and generators. The award is given by the Slovenian Science Foundation (SSF) in cooperation with the World Federation of Scientists (WFS).

Eva Vidak, Young Investigator Award Nomination: Best Speaker at 38th Winter School on proteinases and their inhibitors, ASBMB virtual conference, Identification of extracellular substrates of caspases 3, 7, and 1.

Abida Zahirović, Krka Prize with special recognition for PhD thesis, Novo mesto, Krka, Identification and characterization of major bee venom allergen Api m 1 mimotopes for development of specific immunotherapy.

Andrej Žohar, Best Poster Award, Bled, "30th International Conference Nuclear Energy for New Europe – NENE 2021", September 2021, poster "Silicon carbide neutron detector development computational support with MCNP"

INSTITUTE COLLOQUIA

March 22, 2021: **Nives Ogrinc** (virtual)
Jožef Stefan Institute and Jožef Stefan International Postgraduate School
Stable isotopes in interdisciplinary research

March 23, 2021: **Barbara Malič** (virtual)
Jožef Stefan Institute and Jožef Stefan International Postgraduate School
Ferroelectric ceramics: an overview of a century of research from the discovery of the ferroelectric effect to the present day

March 23, 2021: **David S. Weiss** (virtual)
Pennsylvania State University, University Park, USA
Quantum computing with atoms trapped by light

March 25, 2021: **Janko Petrovčič** (virtual)
Jožef Stefan Institute
Challenges of the development of electronics as a companion of modern research and applications

March 25, 2021: **Andrej Filipčič and Marko Zavrtanik** (virtual)
Jožef Stefan Institute and University of Nova Gorica
Measurements of cosmic particles of extreme energies at the Pierre Auger Observatory

March 26, 2021: **Denis Arčon** (virtual)
Jožef Stefan Institute and Faculty of Mathematics and Physics, University of Ljubljana
Fullerenes: superconductivity, magnetism and qubits

April 14, 2021: **Mitja Luštrek** (virtual)
Jožef Stefan Institute
Optimization of measures to contain the COVID-19 epidemic

April 16, 2021: **Dušan Turk** (virtual)
Jožef Stefan Institute
X-ray diffraction screening of major protease crystals reveals SARS-CoV-2 inhibitors

April 21, 2021: **Claudio Masciovecchio** (virtual)
Elettra Sincrotrone Trieste, Italy
New research opportunities with free electron lasers

May 12, 2021: **Matjaž Leskovar** (virtual)
Jožef Stefan Institute
Modelling of the COVID-19 epidemic in Slovenia

October 27, 2021: **Saša Svetina** (virtual)
Institute of Biophysics, Faculty of Medicine, University of Ljubljana and Jožef Stefan Institute
Why the Nobel Prize for the discovery of the Piezo1 and Piezo2 proteins was awarded

November 24, 2021: **Matej Praprotnik**
National Institute of Chemistry and Faculty of Mathematics and Physics, University of Ljubljana
Multiscale simulations of open molecular systems

December 15, 2021: **Matevž Dular** (virtual)
Faculty of Mechanical Engineering, University of Ljubljana
Cavitation – the path from its prevention to its use for destroying viruses and bacteria

KNOWLEDGE TRANSFER

The JSI pays a lot of attention to furthering its links with industry. In keeping with European aims and the objectives of the Slovenian government, the JSI organized several important meetings on the subject of cooperation with enterprises and industry. In this way the JSI introduced a new method of cooperation, showing industry and the public that it is aware of its leading role, not only in research but also in the transfer of knowledge into practice.

R & D PROJECT PARTNERS

1. Administration of the Republic of Slovenia for Food Safety, Veterinary Sector and Plant Protection, Ljubljana
2. Agency for Radwaste Management, Krško
3. AMZS d.d., Ljubljana
4. A-ROSSO Sašo Cuder s.p., Ljubljana
5. AUDAX d.o.o., Ljubljana
6. BORZEN, Slovenian Power Market Operator, Ljubljana
7. BTT Tekstil d.o.o., Zgornja Kungota
8. Cankarjev dom, Ljubljana
9. Časnik Finance, d.o.o., Ljubljana
10. Cestel d.o.o., Ljubljana
11. Comland d.o.o., Ljubljana
12. Cosylab d.d., Ljubljana
13. Deos, d.o.o., Notranje Gorice
14. Digital Innovation Hub Slovenia, Ljubljana
15. Elektro Celje, d.d., Celje
16. Eles, d.o.o., Ljubljana
17. Elrad International, d.o.o., Gornja Radgona
18. Eurofins ERICo Slovenija d.o.o., Velenje
19. GEN energija, d.o.o., Krško
20. Geološki zavod Slovenije, Ljubljana
21. Grid Instruments, d.o.o., Ljubljana-Črnuče
22. Hidex Novo mesto, d.o.o., Novo Mesto
23. Infinite, d.o.o., Limbuš
24. Institute for Water of the Republic of Slovenia, Ljubljana
25. Iskra ISD Technofusion, Kranj
26. Iskra PIO, d.o.o., Šentjernej
27. Izoelektro, d.o.o., Limbuš
28. JP CČN Domžale-Kamnik, d.o.o., Domžale
29. KMAG, KIA Motors Adria Group, Ljubljana
30. Kolektor Mobility, d.o.o., Idrija
31. Komunala Kranj, d.o.o., Kranj
32. Komunala Novo Mesto, d.o.o., Novo Mesto
33. Krško Nuclear Power Plant, Krško
34. LEK, d.d., Ljubljana
35. LTH Castings, d.o.o., Škofja Loka
36. MAHLE Electric Drives Slovenija d.o.o., Šempeter pri Gorici
37. Milan Vidmar Electric Power Research Institute, Ljubljana
38. Ministry of Defence, Ljubljana
39. Ministry of Education, Science and Sport, Ljubljana
40. Ministry of Finance, Ljubljana
41. Ministry of Infrastructure, Ljubljana
42. Ministry of Public Administration, Ljubljana
43. Ministry of the Environment and Spatial Planning, Ljubljana
44. Murexin, d.o.o., Puconci
45. National Education Institute Slovenia, Ljubljana
46. National Institute of Biology, Ljubljana
47. National Institute of Chemistry, Ljubljana
48. Nutrition Institute, Ljubljana
49. Operato, d.o.o., Ljubljana
50. Plinovodi, d.o.o., Ljubljana
51. Proventus, d.o.o., Šempeter Pri Gorici
52. Quintelligence, d.o.o., Ljubljana
53. RLS Merilna tehnika, d.o.o., Komenda
54. Senso4s, d.o.o., Trzin
55. Slovenian Bekeepers Association, Lukovica
56. Slovenian Radiation Protection Administration, Ljubljana
57. Slovensko društvo ljubiteljev kemije, Ljubljana
58. Statistical Office of the Republic of Slovenia, Ljubljana
59. TIK, d.o.o., Kobarid
60. University Medical Centre Ljubljana, Ljubljana
61. University of Ljubljana, Ljubljana
62. University of Maribor, Maribor
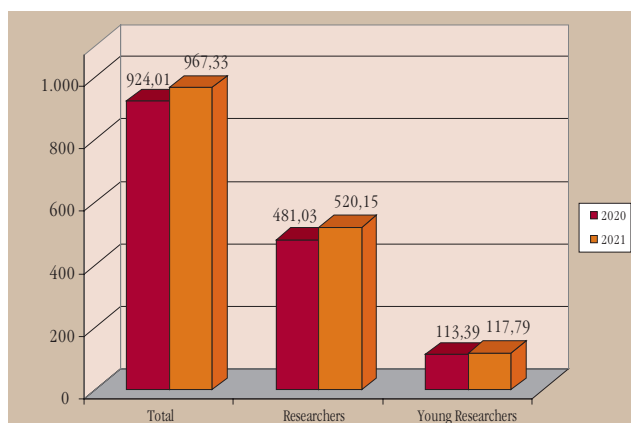63. Zarja elektronika, d.o.o., Kamnik
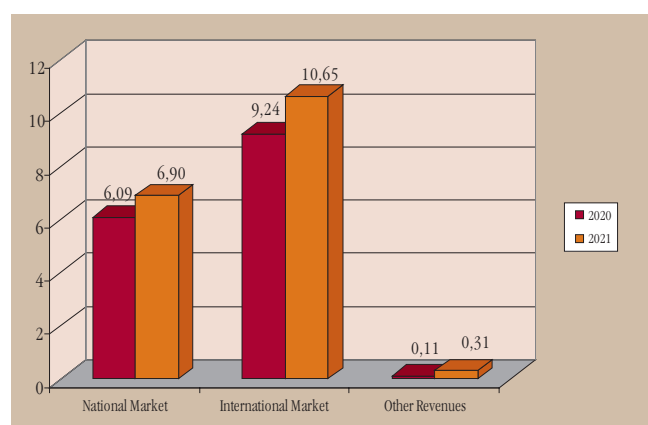
INSTITUTE IN NUMBERS 2020–2021
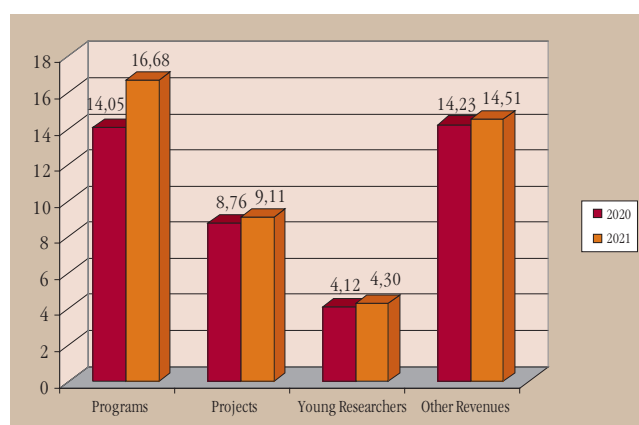
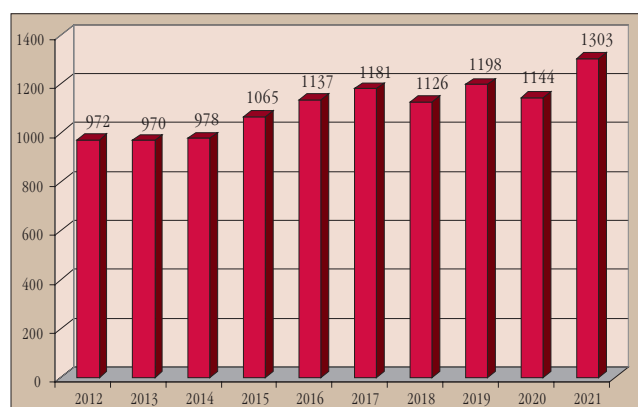## COMPARISON OF REVENUES (€M)
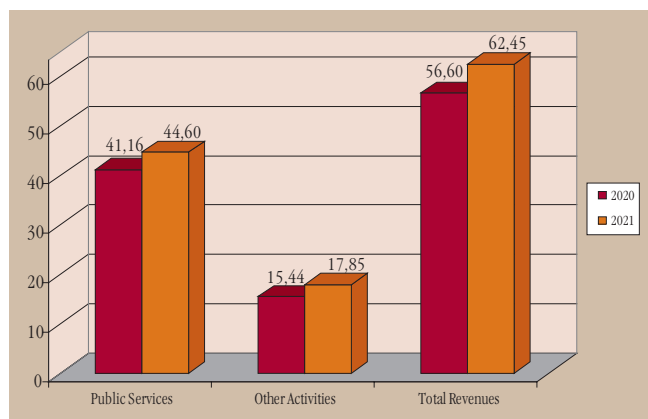
EMPLOYEES (FTE)

REVENUES FROM OTHER ACTIVITIES (€M)

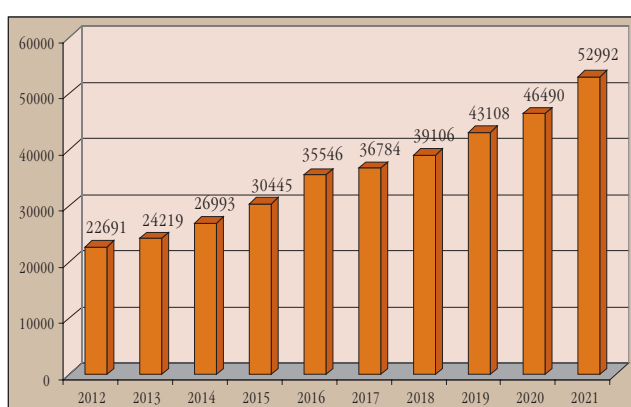## REVENUES FROM PUBLIC SERVICES (€M)

NUMBER OF PUBLICATIONS IN THE WEB OF SCIENCE*

* retrieved 29 November 2022

NUMBER OF CITATIONS IN THE WEB OF SCIENCE*

* retrieved 29 November 2022

RESEARCH DEPARTMENTS

DEPARTMENT OF THEORETICAL PHYSICS F-1

In 2021 members of the programme group THEORY OF NUCLEI, ELEMENTARY PARTICLES AND FIELDS continued with research in the area of hadronic physics, quantum chromodynamics, effective field theory of electroweak decays of mesons, unified theory and precise calculation in three-body systems

Using quantum field theory on the lattice, we extracted the coupled-channel scattering matrix in the charmonium system for the first time. This reproduced the measured properties of the conventional charmonia and rendered predictions for two exotic molecular-like hadrons near the $D\underline{D}$ and $D_s\underline{D}_s$ thresholds, that received support also from experiments. We extracted a resonance in composite Higgs models by simulating the scattering for the first time. The static potentials for the system $\underline{bb}\underline{d}u$ relevant for Z_b resonances have been extracted in all quantum channels.

We proposed a novel method to probe the persistent hints of lepton-flavour universality violation observed in semileptonic B decays. Relying on the specific properties of the Belle II experiment, it consists of comparing the inclusive rates of $\Upsilon(4S)$ into final states with oppositely charged leptons of different flavors. In models with scalar leptoquarks that explain the $R_K^{(*)}$ anomaly and possess the maximum CP-odd coupling we have presented additional constraints from B_s meson mixing. We found that there are asymmetric contributions in the production of leptoquarks at the LHC.

We reconsiderd the decays of pseudoscalar mesons (P) to neutrino pairs and possibly additional photons in the presence of (light) Majorana neutrinos. For this purpose we derived a model-independent general parametrization of the neutrino mass matrices with a physically interpretable and irreducible set of parameters. We updated the SM predictions for the branching ratios of B decays to neutrinos (and photons) and discussed the sensitivity of these decays to the neutrino mass and mixing parameters. With international collaborators, we concluded our analysis of the heavy neutral leptons signature at the Belle II experiment and we are performing an extensive study of the phenomenology of neutrino polarizability. We investigated right-handed fermionic massive dark matter in the processes of neutron decay into dark fermion and photon and decay of D-mesons into dark-fermion pairs. The interaction mediator is the colored scalar.

We explored the interplay of New Physics (NP) effects in leptonic (g–2) Higgs boson decays to leptons within the Standard Model Effective Field Theory (SMEFT) framework, including one-loop Renormalization Group (RG) evolution of the Wilson coefficients as well as matching to the observables below the electroweak symmetry breaking scale.

We used machine-learning (ML) and non-ML techniques to study optimized CP -odd observables, directly and maximally sensitive to the CP -odd top quark - Higgs boson interaction at the LHC and prospective future hadron colliders using the final state with a Higgs boson and a top quark pair, followed by semileptonic t decays. We contributed to the review of the LHC Olympics 2020 challenge, including an overview of the competition, a description of the methods deployed in the competition, lessons learned from the experience, and implications for data analyses with future datasets as well as future colliders.

We embarked on an ambitious project to calculate the quantum fluctuations, which constitute a one-loop correction to the false vacuum decay rate at one loop. We managed to find an analytic expression for the semi-classical action in arbitrary dimension, together with higher-order corrections. We investigated the high temperature fate of four-dimensional gauge-Yukawa theories featuring short-distance conformality of either an interacting or

Head:

Prof. Jernej Fesel Kamenik

- **The lattice simulations reproduce the measured properties of the conventional charmonia and rendered predictions for two exotic molecular-like hadrons near thresholds.**
- **We derived a model-independent general parametrization of neutrino-mass matrices with a physically interpretable and irreducible set of parameters.**
- **We demonstrated the power of the SMEFT framework for New Physics phenomenology.**
- **We explicitly constructed UV-free theories with high-temperature symmetry non-restoration of a global symmetry.**
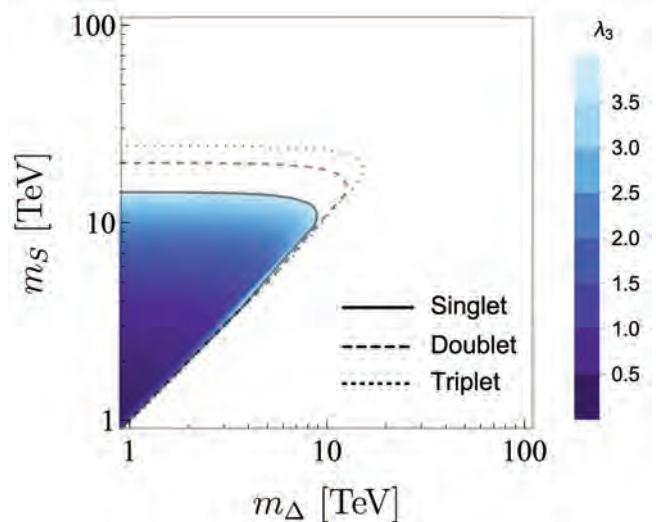

Figure 1: Allowed region of masses of scalar leptoquark and scalar dark matter S for the model to explain the dark-matter abundance in the universe.
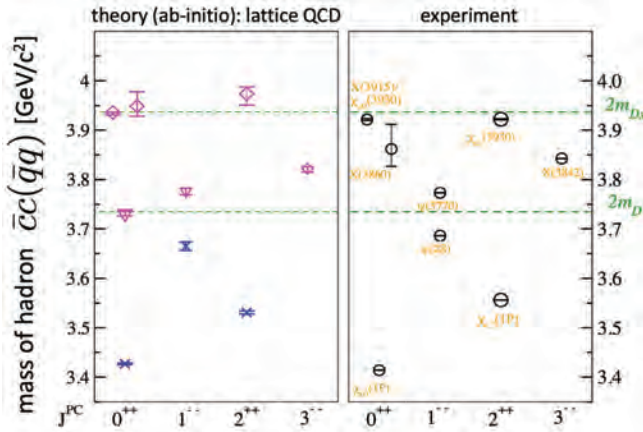
Figure 2: *The lattice simulations roughly reproduce the measured masses of the conventional charmonia and render the predictions for two exotic hadrons near the DD̄ and D̄ₛDₛ thresholds.*

non-interacting nature. We discovered a class of complete asymptotically free theories for which the symmetry breaks at arbitrarily high temperatures. In its minimal form this class is constituted by a theory with two fundamental gauged scalars each gauged under an independent group.

Some outstanding publications in the past year

1. Kasieczka, Gregor, Bortolato, Blaž, Dillon, Barry M., Kamenik, Jernej, Matevc, Andrej, Seljak, Uroš, Smolkovič, Aleks, et al. The LHC Olympics 2020 : a community challenge for anomaly detection in high energy physics. *Reports on Progress in Physics*, ISSN 0034-4885, 2021, vol. 84, no. 12, 124201-1-124201-64, graf. prikazi, tabele, doi: 10.1088/1361-6633/ac36b9. [COBISS.SI-ID 83654915]

2. Fajfer, Svjetlana, Kamenik, Jernej, Tammaro, Michele. Interplay of New Physics effects in (g–2)l and h→l+l− lesons from SMEFT. *The journal of high energy physics*, ISSN 1029-8479, 2021, vol. 2021, no. 6, str. 099-1-099-29, doi: 10.1007/JHEP06(2021)099. [COBISS.SI-ID 67644419]

3. D'Eramo, Francesco, Košnik, Nejc, Pobbe, Federico, Smolkovič, Aleks, Sumensari, Olcyr. Leptoquarks and real singlets: a richer scalar sector behind the origin of dark matter. *Physical review. D*, ISSN 2470-0010, 2021, vol. 104, iss. 1, str. 015035-1-015035-23, ilustr., doi: 10.1103/PhysRevD.104.015035. [COBISS.SI-ID 72243971]

4. Bajc, Borut, Lugo, Adrián, Sannino, Francesco. Asymptotically free and safe fate of symmetry nonrestoration. *Physical review. D*, ISSN 2470-0010, 2021, vol. 103, no. 9, str. 096014-1-096014-20, doi: 10.1103/PhysRevD.103.096014. [COBISS.SI-ID 94731011]

5. Prelovšek, Saša, Collins, Sara, Mohler, Daniel, Padmanath, M., Piemonte, Stefano. Charmonium-like resonances with JPC=0++,2++ in coupled D⁻D,Ds⁻Ds scattering on the lattice. *The journal of high energy physics*, ISSN 1029-8479, Jun. 2021, vol. 2021, art. no. 35, 39 str., ilustr., doi: 10.1007/JHEP06(2021)035. [COBISS.SI-ID 66913795]

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

We continued investigations of transport for disordered quuatum systems. With our numerical method, we upgraded existing results for the Anderson model's conductivity, particularly in the vicinity of localization transition in higher dimensions. Using the rate equations of many-body states we found an analogy of the phenomenon of many-body localization to the percolation problem. Within the theory of integrable quantum lattice models we showed that the macroscopic degeneracy in the noninteracting model leads to a jump in the transport stiffness when the interaction is introduced. We found that the dynamical response of such spin models exhibits an anomalous behaviour in the vicinity of specific values of interaction. We continued studies of frustrated spin systems by evaluating the dynamical correlations in the Kagome lattice, in relation to experiments on real materials.

Within the framework of electron-phonon coupling, we have computed the electron spectral function in disperzive optical phonons. At large optical phonon dispersion, multi phonon states appear at smaller energies then single phonon excitations.

We studied the origin of anomalous dynamics and slow thermalization in quantum spin chains with disorder. We introduced a new approach that describes their properties due to the proximity to conserved quantities of the
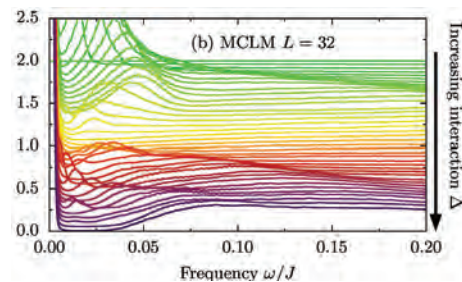

Figure 3: *Dynamical spin conductivity within the Heisenberg spin chain for different values of anisotropy.*
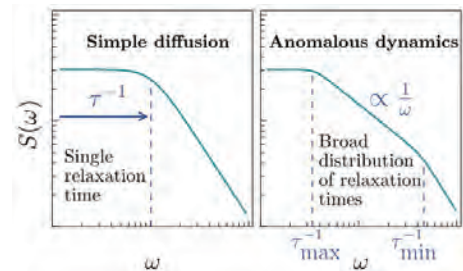

Figure 4: *Behaviour of the spectral function in the case of simple diffusion (left) and anomalous dynamics (right).*

Anderson insulator. This approach allows for a quantitative description of spectral functions of experimentally relevant observables.

We studied the spin Seebeck effect in the Hubbard model on a square lattice. We determined that in the Mott insulator at finite magnetization the spin Seebeck coefficient is anomalously large and by far exceeds thermodynamic estimates, e.g., Heike's and Kelvin's. We explained that the origin for this is in the gap in one particle spectra and the different scattering rates of spins up compared to spins down. We also showed that despite being anomalous, the Seebeck coefficient does not explain the discrepancy between recent cold-atom experiments and theoretical calculations.

In collaboration with an ETH Zurich group we have investigated how the exotic states, such as the generalized Gibbs ensembles can be realized with trapped ions experiments. We obtained two QuantERA projects involving international consortia, which will start with a collaboration in 2022.

Within the framework of excitonic insulators we have discovered a series of new phenomena, including a higher-order Josephson junction, ballistic transport and a photovoltaic effect in the bulk. We developed a new generation of theoretical methods for quantum many-body systems out-of-equilibrium, which will allow a direct comparison with experiments.

We proposed a new model for describing hybrid superconductor-semiconductor devices, where the active components are a superconducting island and a quantum dot. We have devised a method for solving this problem and in collaboration with an experimental group demonstrated that the model is an adequate description of real devices. We have extended the theory of non-trivial Fermi liquids to the multi-orbital case in the presence of an external field, which has allowed us to show that iron phthalocyanine on the surface of gold exhibits a topological transition into a Fermi liquid that is of the non-Landau type. We have shown that the correlated electrons systems exhibit high-temperature universal transport oscillations as a function of magnetic field, which indicates the type of interactions between charge carriers.

Using the Lindblad master equation, we studied a quantum harmonic oscillator coupled to a thermal bath in the presence of a spin-orbit interaction. We found an analytical expression for the asymptotic dynamics of the spin observables. We studied the topological properties of Josephson's junctions in the presence of the Rashba interaction. When the superconducting phase difference equals pi, the band structure of the Andreev bound states may host Dirac points. Such a junction thus behaves as a one-dimensional topological insulator.

We have investigated collective dynamic behaviour in the presence of higher-order interactions enabled by network geometry with simplicial complexes of different dimensions. These structures were generated using the cooperative self-assembly model developed in the previous period. We have shown that triple interactions embedded in triangles lead to the opening of the hysteresis loop and a significantly changed course of the synchronization process between phases caused by the leading pairwise couplings. In the magnetization reversal processes with an external field, the presence of tri-spin interactions on embedded triangles causes hysteresis-loop asymmetry, while the characteristics of magnetization fluctuations remain stable. We have shown, among other results, that collective fluctuations of magnetization on simplicial complexes have the characteristics of self-organized criticality. This behaviour originates in antiferromagnetic interactions that cause spin frustrations on triangular sub-simplexes. Within the microscopic model introduced in 2020, we continued research into the stochastic processes behind the spread of the SARS-Cov_2 epidemic. Based on the high temporal resolution in this model, we were able to determine the impact of asymptomatic virus carriers on the course of the epidemic.

- **We introduced a new approach that describes anomalous dynamics and slow thermalization in quantum spin chains with disorder due to the proximity to conserved quantities of the Anderson insulator.**
- **The Spin Seebeck coefficient in the Hubbard model with finite magnetization exceeds the thermodynamic estimates.**
- **We propose a higher-order Josephson effect in a stack of thin semiconductors.**
- **We developed a methodology for theoretical studies of hybrid devices composed of superconducting islands and quantum dots.**
- **We found an asymptotic solution for the decoherence of a harmonic oscillator in the presence of a spin-orbit interaction.**
- **High-temporal resolution and individual actor's features capture the role of asymptomatic virus carries in the epidemic spreading.**
- **Emerging collective dynamic behaviours in complex systems are based on a geometry that provides contacts of different orders.**
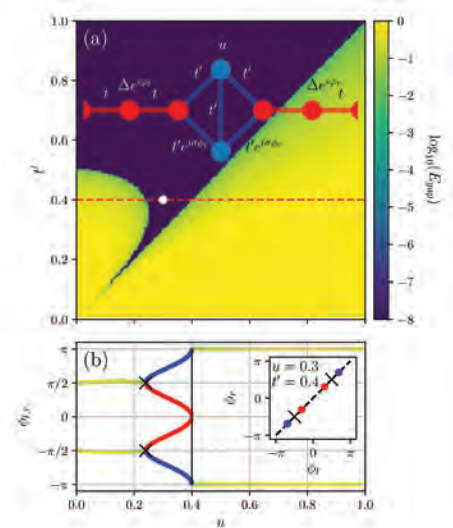

Figure 5: Formation of Dirac points in the band structure of the Andreev bound states in a Josephson junction with Rashba interaction.

Some outstanding publications in the past year

1. Vidmar, Lev, Krajewski, Bartosz, Bonča, Janez, Mierzejewski, Marcin. Phenomenology of spectral functions in disordered spin chains at infinite temperature. *Physical review letters*. [Print ed.]. 2021, vol. 127, iss. 23, str. 230603-1-230603-7, ilustr. ISSN 0031-9007. DOI: 10.1103/PhysRevLett.127.230603. [COBISS. SI-ID 92221699]
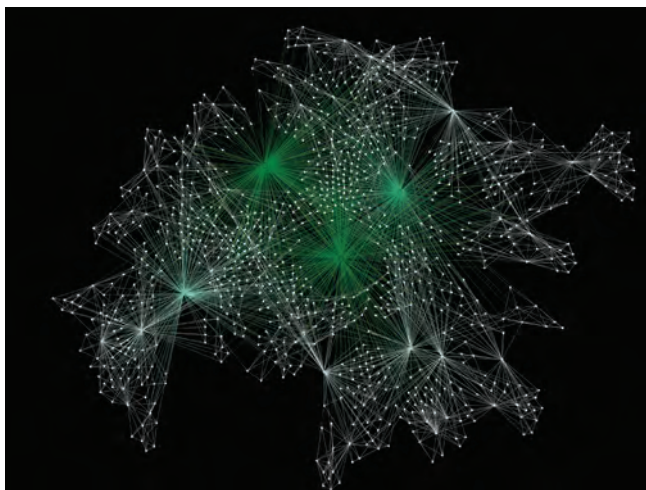
Figure 6: Four-dimensional simplicial complex of self-assembled 5-cliques used in the study of phase synchronization

2. Ulaga, Martin, Mravlje, Jernej, Kokalj, Jure. Spin diffusion and spin conductivity in the two-dimensional Hubbard model. *Physical review. B*, ISSN 2469-9950, 2021, vol. 103, no. 15, str. 155123-1-155123-8, doi: 10.1103/PhysRevB.103.155123. [COBISS.SI-ID 95086851]

3. Reiter, Florentin, Lange, Florian, Shreyans, Jain, Grau, Matt, Home, Jonathan, Lenarčič, Zala. Engineering generalized Gibbs ensembles with trapped ions. *Physical review research*, ISSN 2643-1564, 2021, vol. 3, no. 3, str. 033142-1-033142-18, doi: 10.1103/PhysRevResearch.3.033142. [COBISS.SI-ID 94027011]

4. Pavešić, Luka, Bauernfeind, Daniel, Žitko, Rok. Subgap states in super-conducting islands. *Physical review. B*, ISSN 2469-9950, 2021, vol. 104, no. 24, str. L241409-1-L241409-7, doi: 10.1103/PhysRevB.104.L241409. [COBISS.SI-ID 91146243]

5. Tadić, Bosiljka, Melnik, Roderick. Self-organised critical dynamics as a key to fundamental features of complexity in physical, biological, and social networks. *Dynamics*, 2021, vol. 1, no. 2, str. 181-197, doi: 10.3390/dynamics1020011. [COBISS.SI-ID 82533123]

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

The work of the group for THEORETICAL BIOPHYSICS AND SOFT MATTER PHYSICS investigated various question at the molecular and cellular level.

At the molecular level we studied the spontaneous curvature of two-component lipid systems that form inverted hexagonal phases, and we showed experimentally and theoretically that it does not depend only on concentration but also on the physical dimensions of the molecules. We also used classical molecular dynamics simulations with a polarizable core-shell model for the gold atoms to demonstrate significant effects of explicit metal polarizability on gold nanoparticle solvation and electrostatic properties in aqueous electrolytes. Combining X-ray scattering and molecular simulations, we also showed that glyco-surfactants, which form stable foams, are stabilized by hydrogen bonds. Furthermore, using computer simulations, we studied how the size of the molecule, its shape, and its chemical character affect the sorption and diffusion of the molecule through dense polymer structures. These findings are helpful in developing soft functional materials for biomedical, pharmaceutical, and nano-catalysis applications.

- **We showed that the better absorbed the molecules in a given gel, the slower they diffuse, which means that the permeability only weakly depends on the type of molecule.**
- **We proposed a theoretical description of cell-junctions mechanics in epithelial tissues.**
- **We discovered a photonic band gap in double-twisted structures of liquid crystals formed by achiral molecules.**

Figure 7: Cell rearrangements in epithelial tissues are driven by active forces at cell-cell junctions.

At the level of cells, we analysed the morphologies of compressed model epithelial tissues and we found that the characteristic villus morphologies form only if the cell-level activity is strong enough. We also studied nonlinear dynamics of cell-cell junctions and characterized various types of behaviours, which may significantly contribute to large scale processes such as morphogenesis, tissue repair, and disease. We proposed a theoretical description in which the cell- and tissue-scale mechanics are described within the well-established vertex-model framework, whereas the kinetics of force producing molecules are captured by a set of rate equations. This system describes a mechano-chemical feedback loop, which gives rise to a rich set of junctional behaviours.

A large part of the work over the previous year was dedicated to research related to SARS-CoV-2: We published an extensive review article on the physical mechanisms behind the aerosol transmission of pathogens, with a particular focus on relative humidity. We furthermore investigated in detail the nature of electrostatic interactions between the novel coronavirus and a charged electret layer, taking into account as well the effects of charge regulation. We also studied the role of RNA structure in its interaction with a substrate, which is crucial not only for the assembly and disassembly of RNA viruses but also in nanoparticles used for RNA-based drug delivery.

We studied systems of liquid crystals, where we examined layered structures of bent-core-shaped achiral molecules. We showed that they form a structure in which the long molecular axes rotate from layer to layer, forming a helical structure with a period of four smectic layers. On top of this, another helix is superimposed, the pitch of

which depends on the temperature. We have furthermore investigated the effects of chiral dopands on dynamics of achiral polar smectics. Because of chiral interactions, gaps in relaxation modes appear. Relaxation modes are oppositely chiral in pairs and couple with a chiral field of dopant different for opposite chiralities.

Some outstanding publications in the past year

1. Kanduč, Matej, Kim, Won Kyu, Roa, Rafael, Dzubiella, Joachim. How the shape and chemistry of molecular penetrants control responsive hydrogel permeability. *ACS nano*, ISSN 1936-0851, 2021, vol. 15, no. 1, str. 614-624, doi: 10.1021/acsnano.0c06319. [COBISS.SI-ID 48676867]

2. Alsous, Jasmin Imran, Rozman, Jan, Marmion, Robert A., Košmrlj, Andrej, Shvartsman, Stanislav Y. Clonal dominance in excitable cell networks. *Nature physics*. [Online ed.]. 2022, vol. 17, str. 1391-1395. ISSN 1745-2481. doi: 10.1038/s41567-021-01383-0. [COBISS.SI-ID 95126787]

3. Krajnc, Matej, Stern, Tomer, Zankoc, Clément. Active instability and nonlinear dynamics of cell-cell junctions. *Physical review letters*, ISSN 0031-9007. [Print ed.], 2021, vol. 127, no. 19, str. 198103-1-198103-6, doi: 10.1103/PhysRevLett.127.198103. [COBISS.SI-ID 84201731]

4. Pociecha, Damian, Vaupotič, Nataša, Majewska, Magdalena, Cruickshank, Ewan, Walker, Rebecca, Storey, John M. D., Imrie, Corrie T., Wang, Cheng, Górecka, Ewa. Photonic bandgap in achiral liquid crystals – a twist on a twist. *Advanced materials*, ISSN 1521-4095. [Online ed.], 2021, vol. 33, no. 39, str. 2103288-1-2103288-7, doi: 10.1002/adma.202103288. [COBISS.SI-ID 80061955]
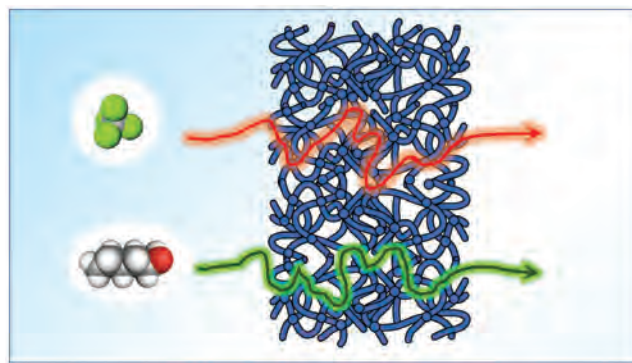

Figure 8: Permeation of molecules through a polymer hydrogel depends on their sorption and diffusion.

Awards and appointments

1. Dr Matej Kanduč: Zois Award for significant scientific achievements in hydration and thermoresponsive hydrogel research, Slovenia.

2. Prof. Dr Nataša Vaupotič: Zois distinction for research in the field of modelling of structures and resonant response of multidimensional thermotropic phases, Slovenia.

Organization of conferences, congresses and meetings

1. International workshop: Quantum many-body dynamics: Thermalization and its violations
2. Institute for basic science (PCS-IBS), Daejeon, South Korea, 24.-28. 5. 2021 (virtual)
3. New generation in strongly correlated systems - NGSCES2021, 7.-10. 6. 2021 (virtual)
4. International workshop: Quantum many-body dynamics: Thermalization and its violations (virtual)
5. Izbrana poglavja v visoko energetski fiziki, astrofiziki in kozmologiji, Medana, Slovenia, 31.5.-2.6.2021
6. Physics of the Flavourful Universe, Portorož, Slovenia, 21.-24.9.2021
7. 4th Trilateral meeting, Ljubljana, 16. 12. 2021
8. Nonequilibrium Quantum Workshop, Krvavec, Slovenia, 12.-16. 12. 2021

INTERNATIONAL PROJECTS

1. Organization of Meeting on „Physics of the flavourful Universe"
   Asst. Prof. Miha Nemevšek
   Cost Association Aisbl
2. COST CA16201; Unraveling New Physics at the LHC through the Precision Frontier
   Asst. Prof. Miha Nemevšek
   Cost Association Aisbl
3. COST CA17139; European Topology Interdisciplinary Action
   Dr. Anže Rapoš Božič
   Cost Association Aisbl
4. International Scientific Workshop: Physics of the Flavourful Universe, Portorož, Slovenia, from 21 September 2021 to 24 September 2021
   Prof. Jernej Fesel Kamenik
   Cost Association Aisbl
5. The Flavor of the Invisible Universe
   Asst. Prof. Nejc Košnik
   Slovenian Research Agency

6. New Searches for Physics Beyond the Standard Model
   Prof. Jernej Fesel Kamenik
   Slovenian Research Agency
7. Manifestation of Quantum Chaos in Quantum Many-Body Lattice Systems
   Asst. Prof. Lev Vidmar
   Slovenian Research Agency
8. The Flavor of Elementary Particles Beyond the Standard Model
   Asst. Prof. Nejc Košnik
   Slovenian Research Agency

RESEARCH PROGRAMMES

1. Theory of the condensed matter and statistical physics
   Prof. Janez Bonča
2. Theoretical physics of nuclei, particles and fields
   Prof. Jernej Fesel Kamenik

3. Biophysics of polymers, membranes, gels, colloids and cells
Prof. Primož Ziherl

R & D GRANTS AND CONTRACTS

1. Orientational Interactions in a Generalized Thomson Problem: Dipole-Stabilized Spherical Nanocontainers
Dr. Anže Rapoš Božič
2. Slow thermalization in quantum many-body systems
Prof. Peter Prelovšek
3. Diagnosing nonequilibrium quantum matter
Asst. Prof. Lev Vidmar
4. The influence of additives on nanoscopic wetting
Dr. Matej Kanduč
5. Multi-scale modeling of non-equilibrium quantum materials
Dr. Denis Golež
6. Three advances towards realistic description of strongly correlated electron transport
Asst. Prof. Jernej Mravlje
7. Symmetries and quantum pumping
Dr. Zala Lenarčič

8. Diamond-assisted quantum processing of fullerene qubits
Prof. Rok Žitko
9. Coulombic subgap states in superconducting quantum devices
Prof. Rok Žitko
10. Nonlinear mechanics of biological tissues and their tumors
Dr. Matej Krajnc
11. Advancing precision flavour studies with machine learning
Prof. Jernej Fesel Kamenik
12. Lattice QCD study of electroweak transitions between heavy mesons and light hadronic resonances (raziskovalni projekt - Program AD)
Dr. Luka Leskovec
13. Cryptographically secure random number generator
Prof. Rok Žitko
14. Financing of projects visits at the Slovenian higher education institutions
Nevenka Hauschild
Public Scholarship, Development, Disability and Maintenance Fund of the Republic of Slovenia
15. Cryptographically secure random number generator
Prof. Rok Žitko
Government Office for the Protection of Classified Information

VISITORS FROM ABROAD

1. Dr Lorenzo Ubaldi, SISSA, Trieste, Italy, 11. 1.-11. 4. 2021, 7.-17. 6. 2021, 26. 7.-1. 8. 2021 and 6. 9. – 21. 9. 2021
2. Prof. Dr Ilja Doršner, University of Split, Faculty of Electrical Engineering, Mechanical Engineering and Naval Architecture, Split, Croatia, 27.-28. 2. 2021, 13. 6.-4. 7. 2021 and 15.-17. 12. 2021
3. Prof. Dr Jure Zupan, University of Cincinnati, Cincinnati, USA, 8. 7.-8. 8. 2021
4. Rafal Swietek, Wroclaw University of Science and Technology, Wroclaw, Poland, 27. 7.-29. 9. 2021
5. Maksymilian Kliczkowski, University of Science and Technology, Wroclaw, Poland, 27. 7.-29. 9. 2021

6. Dr Jacek Herbrych, Wroclaw University of Science and Technology, Wroclaw, Poland, 13.- 24. 9. 2021
7. Dr Patrycja Lydzba, Wroclaw University of Science and Technology, Wroclaw, Poland, 13.- 24. 9. 2021
8. Dr Richard Ruiz, Institute of Nuclear Physics Academy of Science, Krakow, Poland, 25.-29. 9. 2021
9. Dr Toshikaze Chiba, Tohoku University, Sendai, Japan, 17. 10. 2021 – 10. 1. 2022
10. Prof. Dr Damir Bećirević, CNRS/IN2P3 et Université Paris-Saclay, Paris, France, 12.-19. 10. 2021 in 24. 10.-9. 11. 2021
11. Prof. Dr Jure Zupan, University of Cincinnati, USA, 6.-11. 12. 2021
12. Dr Elena Venturini, Technische Universität, Munich Germany, 15.-16. 12. 2021

STAFF

Researchers
1. Dr. Lamprini Athanasopoulou
2. Prof. Borut Bajc
3. Dr. German Gabriel Blesio
4. Prof. Janez Bonča*
5. Dr. Banhi Chatterjee
6. Dr. Luis Cort Barrada
7. Prof. Mojca Čepič*
8. Dr. Ilja Doršner
9. Prof. Svjetlana Fajfer
10. **Prof. Jernej Fesel Kamenik, Head**
11. Dr. Szczepan Glodzik
12. Dr. Denis Golež
13. Dr. Miroslav Hopjan
14. Dr. Matej Kanduč
15. Asst. Prof. Jure Kokalj*
16. Asst. Prof. Nejc Košnik
17. Dr. Matej Krajnc
18. *Dr. Rajmund Krivec, retired 01.10.21*
19. Dr. Zala Lenarčič
20. Dr. Luka Leskovec
21. Asst. Prof. Jernej Mravlje
22. Dr. Sourav Nandy
23. Asst. Prof. Miha Nemevšek
24. Prof. Peter Prelovšek
25. Prof. Saša Prelovšek Komelj
26. Prof. Anton Ramšak*
27. Dr. Anže Rapoš Božič
28. Asst. Prof. Tomaž Rejec*
29. Prof. Bosiljka Tadić

30. Dr. Michele Tammaro
31. Horacio Andres Vargas Guzman, B. Sc.
32. Prof. Nataša Vaupotič*
33. Asst. Prof. Lev Vidmar
34. Prof. Primož Ziherl*
35. Prof. Rok Žitko

Postdoctoral associates
36. Dr. Fabio Staniscia
37. Dr. Clement Adrien Zankoc

Postgraduates
38. Blaž Bortolato, B. Sc.
39. *Victor Francisco Guada Escalona, B. Sc., left 01.04.21*
40. Arman Korajac, M. Sc.
41. Marco Matteini, M. Sc.
42. Luka Medic, B. Sc.
43. Luka Pavešić, B. Sc.
44. Jan Rozman, B. Sc.
45. *Dr. Aleks Smolkovič, left 01.10.21*
46. Rafal Piotr Swietek, M. Sc.
47. Marin Šako, M. Sc.
48. Jan Šuntajs, B. Sc.
49. Martin Ulaga, B. Sc.
50. Iris Ulčakar, B. Sc.

Technical and administrative staff
51. Nevenka Hauschild

Note:

* part-time JSI member

BIBLIOGRAPHY

ORIGINAL ARTICLE

1. Matej Kanduč, Won Kyu Kim, Rafael Roa, Joachim Dzubiella, "How the shape and chemistry of molecular penetrants control responsive hydrogel permeability", *ACS nano*, 2021, **15**, 1, 614-624.
2. Zhujie Li, Victor G. Ruiz, Matej Kanduč, Joachim Dzubiella, "Highly heterogeneous polarization and solvation of gold nanoparticles in aqueous electrolytes", *ACS nano*, 2021, **15**, 8, 13155–13165.
3. Simon Poblete, Anže Lošdorfer Božič, Matej Kanduč, Rudolf Podgornik, Horacio V. Guzman, "RNA secondary structures regulate adsorption of fragments onto flat substrates", *ACS omega*, 2021, **6**, 48, 32823–32831.
4. Damian Pociecha, Nataša Vaupotič, Magdalena Majewska, Ewan Cruickshank, Rebecca Walker, John M. D. Storey, Corrie T. Imrie, Cheng Wang, Ewa Górecka, "Photonic bandgap in achiral liquid crystals - a twist on a twist", *Advanced materials*, 2021, **33**, 39, 2103288.
5. Jan Šuntajs, Tomaž Prosen, Lev Vidmar, "Spectral properties of three-dimensional Anderson model", *Annals of physics*, 2021, **435**, 2, 168469.
6. Michael Kaltenegger, Johannes Kremser, Moritz P. K. Frewein, Primož Ziherl, Douwe Bonthuis, Georg Pabst, "Intrinsic lipid curvatures of mammalian plasma membrane outer leaflet lipids and ceramides", *Biochimica et biophysica acta. Biomembranes*, 2021, **1863**, 11, 183709.
7. Ivana Štibi, Mojca Čepič, Jerneja Pavlin, "Physics teaching in Croatian elementary and high schools during the Covid-19 pandemic", *CEPS journal: Center for Educational Policy Studies Journal*, 2021, **11**, pos. št., 335-359.
8. Bosiljka Tadić, Roderick Melnik, "Microscopic dynamics modeling unravels the role of asymptomatic virus carriers in SARS-CoV-2 epidemics at the interplay between biological and social factors", *Computers in Biology and Medicine*, 2021, **133**, 104422.
9. Timon Grabovac, Ewa Górecka, Damian Pociecha, Nataša Vaupotič, "Modeling of the resonant X-ray response of a chiral cubic phase", *Crystals*, 2021, **11**, 2, 214.
10. Matej Kanduč, Rafael Roa, Won Kyu Kim, Joachim Dzubiella, "Nanochannels and nanodroplets in polymer membranes controlling ionic transport", *Current opinion in colloid & interface science*, 2021, **56**, 101501.
11. Bosiljka Tadić, Roderick Melnik, "Self-organised critical dynamics as a key to fundamental features of complexity in physical, biological, and social networks", *Dynamics*, 2021, **1**, 2, 181-197.
12. Blaž Bortolato, Jernej Kamenik, "Light Majorana neutrinos in (semi)invisible meson decays", *The European physical journal. C*, 2021, **81**, 5, 388.
13. Jan Rozman, Matej Krajnc, Primož Ziherl, "Morphologies of compressed active epithelial monolayers", *The European physical journal. E, Soft matter*, 2021, **44**, 7, 99.
14. Bosiljka Tadić, Neelima Gupte, "Hidden geometry and dynamics of complex networks: spin reversal in nanoassemblies with pairwise and triangle-based interactions", *Europhysics letters*, 2021, **132**, 6, 60008.
15. Dina Jukić, Mojca Čepič, "Temperature ranges of the chiral polar smectic phases", *Europhysics letters*, 2021, **133**, 3, 36001.
16. Sebastian Milster, Won Kyu Kim, Matej Kanduč, Joachim Dzubiella, "Tuning the permeability of regular polymeric networks by the cross-link ratio", *The Journal of chemical physics*, 2021, **154**, 15, 154902.
17. Matej Kanduč, Emanuel Schneck, Cosima Stubenrauch, "Intersurfactant H-bonds between head groups of n-dodecyl-β-D-maltoside at the air-water interface", *Journal of colloid and interface science*, 2021, **586**, 588-595.
18. Saša Prelovšek, Sara Collins, Daniel Mohler, M. Padmanath, Stefano Piemonte, "Charmonium-like resonances with $J^{PC} = 0^{++}, 2^{++}$ in coupled $D\bar{D}, D_s\bar{D}_s$ scattering on the lattice", *The journal of high energy physics*, 2021, **2021**, 35.
19. Svjetlana Fajfer, Jernej Kamenik, Michele Tammaro, "Interplay of New Physics effects in $(g-2)_l$ and $h \rightarrow l^+l^-$ lesons from SMEFT", *The journal of high energy physics*, 2021, **2021**, 099.
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DEPARTMENT OF LOW AND MEDIUM ENERGY PHYSICS — F-2

The members of the Department of Low and Intermediate Energy Physics are engaged in the research in the field of atomic, molecular, optical and nuclear physics. A deep understanding of atomic and nuclear processes is paramount in interdisciplinary research conducted at our department, and includes activities in the fields of environmental radiological monitoring, material research, fusion, biology, energy storage, medicine, pharmacology, environmental sciences and archaeometry. Our research is conducted using our own experimental equipment, consisting of an ion-beam accelerator and beamlines, dedicated detectors of ionizing radiation, experimental setups for atomic and molecular physics and calibrated radiation fields.

Head:
Prof. Primož Pelicon

 Researchers from our department are regular users of large experimental research facilities worldwide, such as particle accelerators, synchrotrons and free-electron lasers. These facilities are accessed either through international collaborations, research networks or through self-initiated research proposals. To counterweight the process of engagement of national human resources at research facilities abroad, we are providing transnational access (TNA) to the tandem ion accelerator at the Jožef Stefan Institute and the instrumentation at the beamlines for international users within the EU H2020 RADIATE project.

We were engaged at the three-spectrometer facility of the Mainz Microtron (MAMI), with the focus on analysing the data acquired during recent production runs. The final analysis of our measurements of virtual Compton scattering performed over more than a decade at the A1 Collaboration at MAMI has now yielded the Q2-dependence of generalized proton polarizabilities (*Fonvieille et al., Phys. Rev. C 2021*). We have re-analysed elastic electron scattering on protons at very-low-momentum transfer from the data acquired in the ISR experiment and studied the role of specific models in the extraction of the proton radius, a persistently elusive quantity constituting the so-called "proton radius puzzle"; the final results were published (*Mihovilovič et al., Eur. Phys. J. A. 2021*). Our work in the MAGIX Collaboration at the MESA accelerator under construction encompassed the study of the operation and characterization of a windowless gas jet target in high-intensity electron beams to be used in conjunction with the MAGIX spectrometers (*Schlimme et al., NIM A 2021*) and electron-beam studies of light collection in a scintillating counter with embedded wavelength-shifting fibres (*Lauß et al., NIM A 2021*).

Our work at the Thomas Jefferson National Accelerator Facility (Jefferson Lab) has been focused on an analysis of the data from several experiments performed during the 6-GeV CEBAF era, but we have also new results on data taken with the new 12-GeV beam. We have published our analysis of the generalized spin polarizabilities of the neutron in the low-Q2 region (*Sulkosky et al., Nature Physics 2021*). These observables quantify the neutron's spin precession under electromagnetic fields at very low energy-momentum transfer squared, and in this regime, chiral effective field theory calculations are expected to be applicable. Our data, however, show a strong discrepancy with these predictions, presenting a challenge to the current description of the neutron's spin properties. We also published new results of our measurements of the proton spin structure at long distances (at low Q2) (*Zheng et al., Nature Physics 2021*). Our results show that a complete description of the nucleon spin remains elusive, and calls for further theoretical work, for example, in lattice QCD. We have also shown that our data, when extrapolated to the photon point, agree with the Gerasimov Drell–Hearn sum rule, a fundamental prediction of quantum field theory that relates the anomalous magnetic moment of the proton to its integrated spin-dependent cross-sections. The analyses of our measurements of cross-sections in the Ar(e,e'p) and Ti(e,e'p) processes were also published (*Gu et al., Phys. Rev. C. 2021*).

In parallel with the construction of the FAIR (Facility for Antiproton and Ion Research) accelerator centre, which is one of the largest projects for basic research in the world, the FAIR Phase-0 research programme is already taking place at the GSI premises in Darmstadt. Our primary focus here is the NUSTAR physics programme, devoted
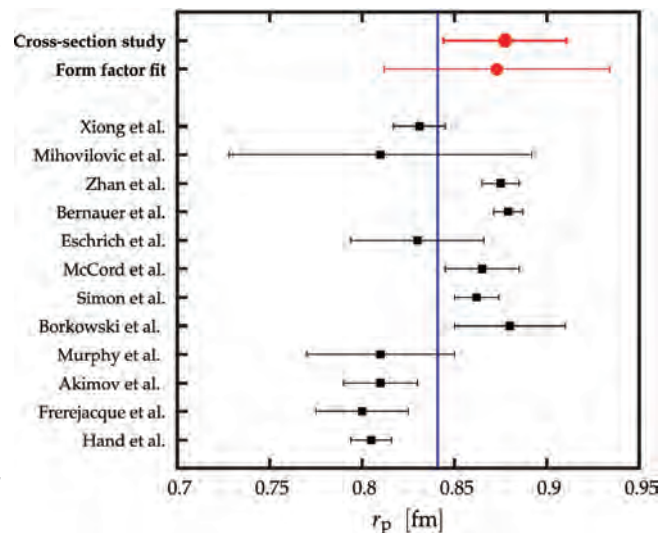

Figure 1: Proton charge radius extracted from electron-scattering experiments. The red circles show the results of the initial-state radiation experiment at Mainz Microtron (Mihovilović et al, Europ. Phys. J. A 57, 107, 2021).
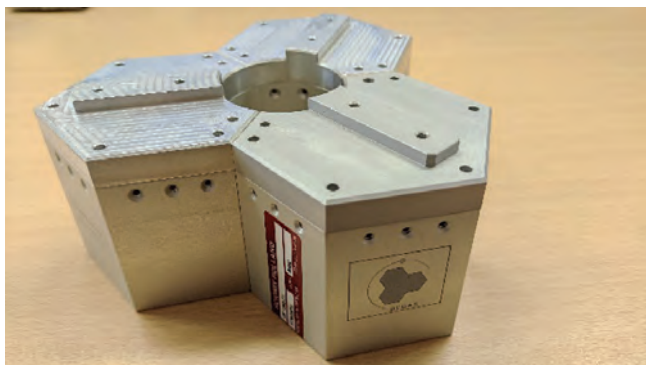
Figure 2: Three BGO scintillation detectors shown the way they will be mounted in the DEGAS spectrometer at FAIR. The detectors were developed at JSI.
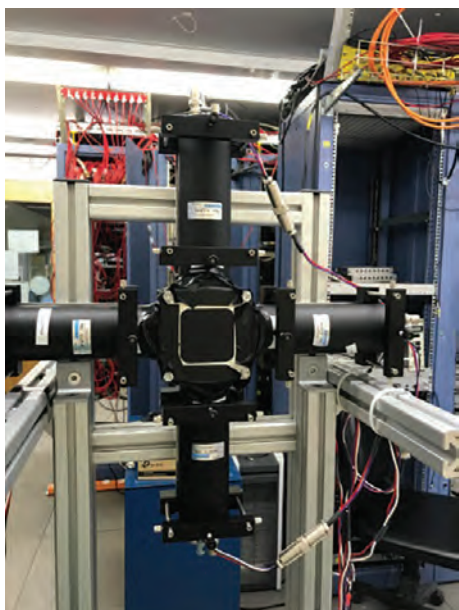

Figure 3: Spatially and temporally resolving detector for implantations and decays of exotic ions at FAIR, where the JSI collaborators contribute their research efforts.
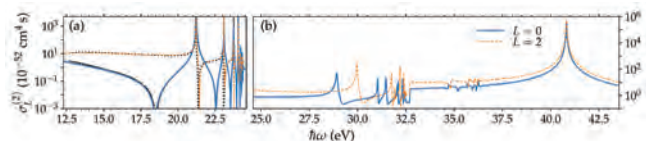

Figure 4: Generalized partial two-photon ionization cross-sections of the helium atom calculated with our novel approach based on exterior complex scaling (A. Mihelič and M. Horvat, PRA 103, 043108, 2021). The total orbital angular momentum of the final state has been denoted by L.

to nuclear structure, reactions and astrophysics, crucial for understanding the creation of all the matter in the universe. We are strongly engaged in the research at the in High-Resolution In-Flight Spectroscopy/ Decay Spectroscopy (HISPEC/DESPEC) and Super Fragment Separator (Super-FRS) sub-collaborations. HISPEC/DESPEC experiments aim to address the key issues in nuclear structure, reactions and nuclear astrophysics at the limits of nuclear existence. We have actively participated in the experiments of the DESPEC collaboration studying the Prolate-Oblate Shape Transition around A~190, 220<A<230 Po-Fr nuclei lying in the south-east frontier of the A~225 island of octupole deformation as well as core-breaking in the most neutron-deficient Sn isotopes.

The new state-of-the-art gamma spectrometer DEGAS (DEspec Germanium Array Spectrometer) is being constructed at GSI/FAIR. When completed, it will incorporate the new BGO scintillation detectors (Figure 2) that we developed as part of the DESPEC collaboration. These detectors are key to ensuring the active shielding of DEGAS against the background noise and Compton scattered photons.

We started the cooperation in the construction of the implantation detector which consists of scintillating fibres. It will be used in experiments of the DESPEC collaboration at GSI/FAIR. We took part in the Super-FRS experiment aiming at fission isomer studies where a superdeformed second minimum in potential energy surface appears in actinides. This is an ideal testing ground for strongly deformed low-spin nuclei and shell corrections in very heavy systems. Our responsibility was the analysis of the FastCom TDC dataset and the modelling of the detection process in the ion implanter (Figure 3). Furthermore, we collaborated in the experiment aimed at direct mass measurements of heavy N=Z and N=Z-1 nuclides to better understand the isospin-symmetry breaking forces for heavier nuclei. We extended the physics model for the ion dynamics simulation framework ITSIM that supports the mass spectrometer optimization and tuning.

In 2021 we were busy with the analysis of the results from the FERMI free electron laser (FEL) experiment, with which we have studied the interference between the $\omega_1+\omega_1$ and $\omega_3-\omega_1$ two-photon pathways, accessible by combining the fundamental (ω_1) with the third harmonic (ω_3) light. We measured the variation of the electron yield in the energy region of the helium $2s^2$ doubly excited state by varying a phase difference between the ω_1 and ω_3 carrier waves. We have performed a detailed first-principles simulation of the process, which has been observed for the first time using only short-wavelength XUV light (a similar technique called RABBITT combines XUV light with IR laser light), and we have submitted a paper to a high-ranking open-access journal. In cooperation with French colleagues from the LCPMR Lab in Paris and based on the analysis of these FERMI results, we ensured a continuation of such coherent control measurements, which have been proposed to verify the operation of the so-called atomic $\omega/3\omega$ interferometer. The latter is expected to provide the unknown phase difference of two-colour light based on a known atomic response to two-photon absorption/emission.

In collaboration with colleagues from XFEL in Hamburg (Germany), we have upgraded the paraxial treatment of self-triggered stimulated emission in the X-ray and XUV energy ranges by introducing a new method for the generation of the spontaneous emission signal via correlation functions. This significantly improves the credibility of modelling the passage of intense light through matter when the duration of the light pulses is not much shorter than the lifetime of an excited state. Based on simulations with an improved accuracy, we proposed new measurements of stimulated emission in helium, intending to use a specially designed gas cell. An oblong glass cell was designed, which will allow the controlled setting of high gas pressure in a limited volume passed by the intense light without any windows present. The cell will be produced by the Laser Laboratory group of the Polytechnic in Milan, with which we have started a collaboration in 2021.

In 2021 we were actively collaborating with the group from the LCLS FEL (A. Halavanau from Stanford, USA), where together with the group from XFEL we participate in the XLO project. We help with the realization of the idea, according to which the self-triggered stimulated emission would be brought back to the target with a delay and via reflection on the crystals, where, together with the next burst of light, the FEL would generate an even stronger burst of stimulated light. Light amplification works similarly for lasers in the visible region, but with the important difference that the lifetime of the excited (upper) state is now much shorter and, therefore, the population inversion

must be generated at each transition in time with a new burst of FEL light. In this project, we collaborate with simulations of the passage of (strong) two-color light through matter (FEL light + return amplified spontaneous emission of the target) performed by our PhD student Špela Krušič.

In collaboration with another XFEL group (L. Mercadier), we participated in one of the first experiments at the new SCS beamline, which is equipped with a spectrometer for measurements in the direction of the incident beam (design by J. Nordgren, J. E. Rubensson, Uppsala University). In this experiment, short pulses of intense XUV light with a photon energy just above the L_3 edge in copper at 933 eV were shot through a 500- and a 100-nm-thick copper foil. A pair of spectrometers measured the spectrum of individual pulses of light in front of and behind the target, and, from this data, the absorption spectrum could be reconstructed for each pulse. Surprisingly, we found that, in a solid target, the generation of photoelectrons and secondary (Auger) electrons is so efficient that it can modify the absorption spectrum of an intense pump light pulse, even though the pulse only lasts a few tens of femtoseconds. Photoelectrons from the nearby copper atoms form holes in the 3d outer shell of the neighbouring atoms and thus open an effective new absorption channel at the characteristic energy of the Lα line transition. The quantitative interpretation of the results of the experiment, which represents the first case of transient absorption with the soft X-ray light, is already underway. To mimic the target environment, it is necessary to simulate plasma development on a short time scale, but under demanding conditions of high target density and high light intensity.

We have devised a theoretical method for the calculation of partial multiphoton ionization amplitudes and cross-sections applicable to atoms and simple molecules (*Mihelič and Horvat, Phys. Rev. A 103, 043108, 2021*). The method, which is based on exterior complex scaling (ECS), can be used to calculate the partial ionization amplitudes for both resonant and non-resonant multiphoton ionization in an efficient way, by analysing the scattered part of the solution of the driven Schrödinger equation in the non-scaled region of space (Figure 4).

At the end of 2021 we took part in two experiments at the Trieste FEL facility, FERMI. In the first experiment we characterized short-lived dipole-allowed [1]P doubly excited resonances in helium using intense, circularly polarized light. Under such experimental conditions, it is likely that an electron from the doubly excited state is knocked out of the atom by the absorption of an additional photon, even before the resonance decays by autoionization with a typical lifetime of a few fs. Thus, transitions to the final excited states of the helium ion He+ with n=2,3,4 were observed, whereby the ratios between the corresponding photoelectron yields reveal the strength of electron-electron correlations in the selected intermediate doubly excited state.

The second experiment was proposed by A. Mihelič, with the goal to investigate to what extent the presence of light resonant with a transition from the ground state to an excited state of the atomic core of a continuum state is able to modify the primary ionization from the atomic ground state. Is the probability that an electron from the primary ionization event would absorb such an additional photon increased? The analysis of the measurements is expected to show whether the process can be distinguished from an analogous process in ionic species.

In the research with twisted light (light that carries orbital angular momentum), led by G. De Ninno of the University of Nova Gorica, we helped to prepare a manuscript in which we demonstrate the possibility to generate and control magnetization in irradiated matter on the nanoscale. The analysis of dichroism observed in the previous experiment at the FERMI FEL, where He atoms were excited to singly excited states with short and highly focused XUV light pulses, and from there to the "rotating" Rydberg states by a pulse of twisted IR light, showed the formation of a localized (on the axis of both light beams) and persistent (having the lifetime of the Rydberg states) magnetic fields generated by the electron current loops of rotating Rydberg wave packets.
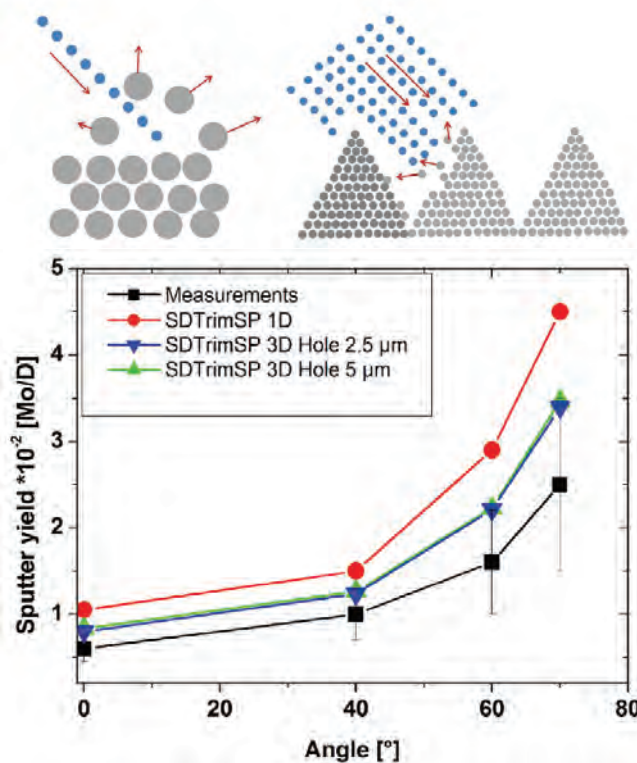

Figure 5: Experimental study on the dependence of sputtering yields with 1-keV deuterium ions under physical conditions in fusion tokamaks. The role of surface roughness is elaborated (Kelemen et al, J. Nucl. Mat. 2021)
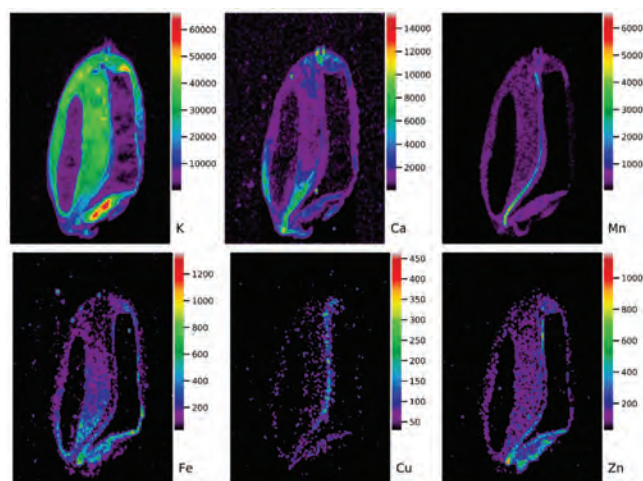

Figure 6: Elemental distribution maps of elements in wheat grain, measured at an upgraded in-air microbeam. The elemental concentrations are presented in ppm.

In September 2021 we concluded a series of X-ray Raman spectroscopy (XRS) measurements to study the redox reaction mechanism of novel redox-active organic materials. The experiment I-20210340 EC took place at the P01 beamline of the PETRA III synchrotron at DESY, Hamburg in collaboration with the Group for Modern Battery Systems from the National Institute for Chemistry. Within the experiment, XRS measurements on batteries based on various organic polymers (PAQS and TB97) in combination with Al anode were performed. The electrochemical mechanism in all studied batteries was confirmed to be a reduction of double carbonyl bond, regardless of the type of organic polymer used in the cathode. Relative amounts of carbonyl bond during battery cycle were quantitatively determined in good agreement with electrochemical values, calculated from the measured capacity.

We have published the results of laboratory characterization of the electrochemical conversion of sulphur in Li-S batteries by measuring X-ray emission spectra (XES). XES measurements were performed at the Microanalytical Centre using MeV proton excitation. The average sulphur charge in the battery cathode was determined from the energy shift of the $K\alpha$ emission line and from the spectral shape of the $K\beta$ emission spectrum (Kavčič et al. *ACS Appl. Energy Mater. 2021, 4, 2357–2364*). An extensive theoretical modelling of the measured XES spectra was used to identify different sulfur compounds and quantitatively determine their relative amounts (Petric et al. *Chem. Commun., 2021, 57, 7573–7576*).
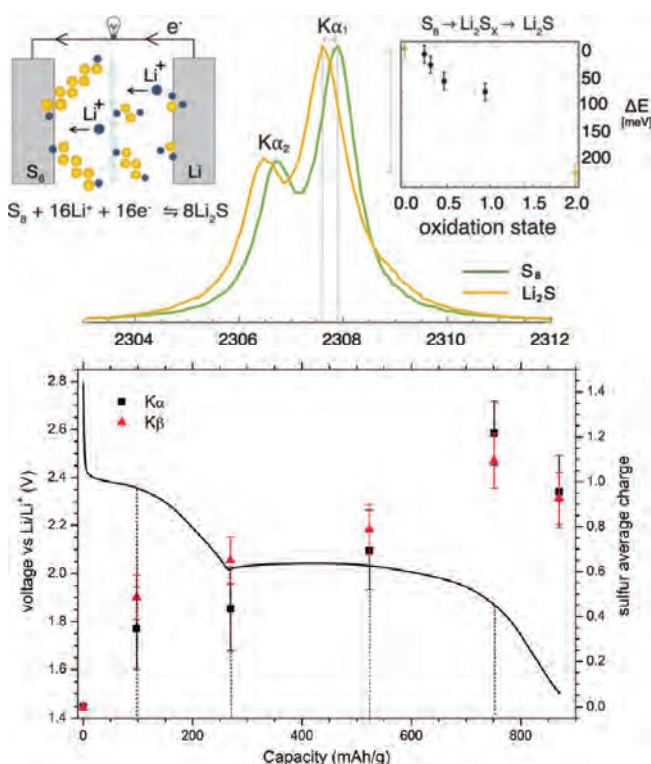

Figure 7: Sulphur average charge in individual battery cathodes stopped at different points during the discharge, as determined from the measured energy shift of the $K\alpha$ emission line and from the changes in the shape of the $K\beta$ emission spectra (From Kavčič et al., ACS APPL. Energy Mat. 2021).

The JSI tandem accelerator provided 4000 beam hours to the users in 2021.

In October and November 2021, we performed a major upgrade of the accelerator and successfully installed a new control system (new communication hardware, new control software).

An extensive upgrade of the external beamline was performed to expand the capabilities of our setup towards in-air measurements of elemental distributions in the sample across a relatively large surface area (~ 1 cm^2) with the lateral resolution of a few tens of μm. We have completed the beam characterization after the upgrade and performed the first quantitative analysis of the distribution of mineral nutrients in plant samples (Figure 6). We constructed and acquired the key components for the new nanobeam beamline, which is to be assembled and tuned by the end of 2022.

We conducted extensive research with the micro-PIXE and MeV-SIMS methods in the field of medicine and biology. With collaborators from the Max Planck Institute for Human Cognitive and Brain Sciences in Leipzig, we showed that the dominant contribution to the transverse relaxation rate in nigrosome 1 originates from iron accumulated in the neuromelanin of dopaminergic neurons. Based on our research, we provided the directions for the development of biomarkers for early detection of dopaminergic neuron depletion in Parkinson's disease. At the JSI we contributed elemental maps of brain tissue measured by micro-PIXE, which revealed quantified distribution of iron in neurons (*Brammerloh et al, Neuroimage 2021*). With a multimodal microscopy approach, combining STED, electron, helium and ion microscopies, we studied the nature of hip prosthesis wear particles and their origin in the periprosthetical tissue (*Podlipec et al, Materials 2021*).

The members of the Infrastructure Group for Ionizing Radiation Measurements conducted the environmental radioactivity monitoring of the living environment in Slovenia, regular Krško Nuclear Power Plant (NPP) off-site environmental radioactivity monitoring, independent verification of the regular environmental radioactivity monitoring around KNPP, monitoring of radioactivity in fodder, central radioactive-waste repository radiological monitoring, monitoring of the radioactivity in drinking water, material characterizations, calibrations of the radiation gauges and the measurements of the personal and environmental doses by thermos-luminescent dosimeters. These activities are accredited according to the SIST EN ISO/IEC 17025 standard. Our results at international round-robin measurements regularly rank as one of the most accurate among the participating institutions. Based on this score, we are often invited to collaborate in groups for characterization and the development of the reference materials.

In accordance with the authorisation, granted by the Slovenian Radiation Protection Administration, 2200 personal dose measurements of exposed workers with thermos-luminescence dosimeters (TLDs) were carried out in 2021. We also carried out ambient dose equivalent measurements with TLDs at 130 different locations. In 2021, 246 calibrations were performed at the NDS (including 159 calibrations of dose rate meters, 50 calibrations of electronic personal dosimeters and 37 calibrations of contamination meters). In addition, 120 dosimeter irradiations

of TL and OSL dosimeters were performed. In total, 744 measurements were made in the LMR laboratory as part of regular programmes for the monitoring of radioactivity in the environment, and 28 measurements were made for sporadic customers. Of these, two were analyses of food imports under the new authorisation of the Ministry of Agriculture and Rural Development (UVHVVR). In 2021, 168 measurements of tritium in water samples were carried out in the framework of radioactivity monitoring in the vicinity of the Krško nuclear power plant (NPP) and in the Republic of Slovenia. For sporadic customers, tritium activity concentrations were determined in 4 samples.

In 2021 we continued intensive collaboration with the Metrology Institute of the Republic of Slovenia (MIRS). As a designated institution and as the holder of the national standard for the field of ionizing radiation, we continued the activities on EU-funded EMRP projects. The members of ISMIS carried out research and development in the field of measurement and analysis methods in gamma spectrometry, thermoluminescence dosimetry and liquid-scintillation spectrometry in the following projects:

- EMPIR 2017 17RPT01 *DOSEtrace - Research Capabilities for Radiation Protection Dosimeters*
- EMPIR 2019, *JNT-w08 supportBSS - Support to the European Metrology Network for reliable legislation in the field of radiation protection*
- PR-02570-1 - *Preparation of reference and intercomparison materials, in cooperation with IARMA*

In 2020 we started sampling and analysing groundwater, thermal waters, precipitation and surface water in the area of influence of hydroelectric power plant (HPP) Mokrice in the framework of the project "*Qualitative and quantitative monitoring of groundwater in the impact area of the dam for HPP Mokrice*". The project is led by IRGO, d.o.o., coordinated by the O2 department at the JSI. NLZOH also participates in the project. The purpose of the project is to determine the state of the environment before the start of construction of HPP Mokrice. Our group participates in the task of determining the concentration activities of H-3 and the total content of alpha and beta emitters in water from boreholes in the construction area of the HPP Mokrice. In 2021, we carried out the planned sampling and analysis of 164 samples.

We continued our studies of the occurrence of organically bound tritium (OBT), tissue free water tritium (TFWT), and C-14 in various terrestrial and aquatic organisms in the vicinity of the NPP and at the reference sites. In 2021, TFWT and OBT were determined in 78 samples. In the research study on the alpha and beta radiant content of drinking water samples in Slovenia, 160 samples were sampled and analysed, and 61 samples were analysed in the study in the influence area of the Mokrice HPP. A total of 84 measurements of C-14 content in water, biota, semi-finished furniture and fuels, and ethanol in its original form and as CO_2 were carried out. In 2021, we did not detect tritium in urine and Ra-226/Ra-228 in water.

In 2021 we purchased a new 320-kV Comet iXRS-320 X-ray machine, which will increase the scope of our activities in the field of X-ray calibrations. We have also purchased the following equipment with the financial support of the Administration of the Republic of Slovenia for Civil Protection and Disaster Relief (ACPDR): a Flir IdentiFINDER portable spectrometer, an Automess dose rate meter, a Berthold neutron dose rate display and a Nuvia WIMP swab meter.

On 26 and 27 October 2021, the Ecological Laboratory with Mobile Unit (ELME) participated, as a part of the Slovenian Protection and Rescue Force, in one of the largest IAEA international exercises in the field of nuclear and radiological emergencies, ConvEx-3b. The exercise was based on an accident at the Barakah nuclear power plant in the United Arab Emirates (UAE). Together with the RS Protection and Rescue Administration and the RS Nuclear Safety Administration, we practiced the use of different communication channels for information exchange and provided international assistance to the affected country through the Response and Assistance Network (RANET) system.

ELME members participated in the 8th International Defence, Security, Safety and Rescue Fair SOBRA 2021 in Gornja Radgona from 23 to 25 September 2021.

In 2021 we started the implementation of the project *The Third NPP Krško Periodic Safety Review Programme, Safety Factor 15 - Radiological Impact on the Environment*, in the Technical Specifications, *No SP-ES1388*. The purpose of the project is to review the adequacy of the documentation in *Safety Factor 15*. Based on the findings of the review, we are making a substantial contribution to the authorisation of the NPP for operation in the next period.
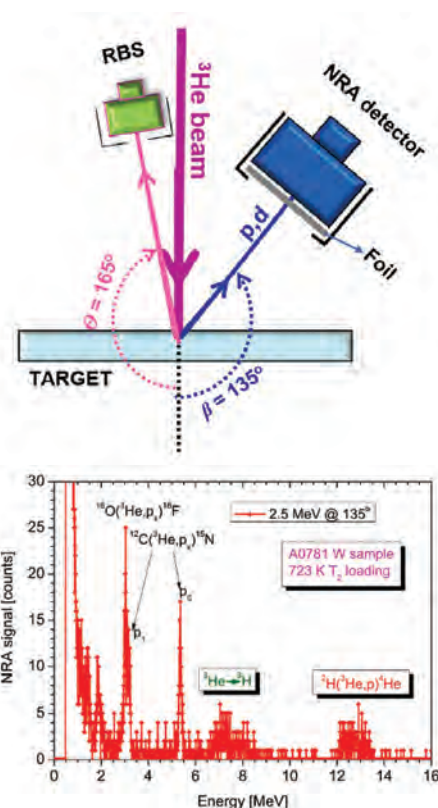

Figure 8: Schematics of the measurement and the identification of nuclear reaction products in the ³He induced nuclear reaction on tritium, in the efforts to apply nuclear reaction analysis with the accelerated ³He ion beam for tritium quantification in materials. The experiments were made in collaboration with CEA, Cadarache (From Markelj et al., Nuclear Materials and Energy 2021).
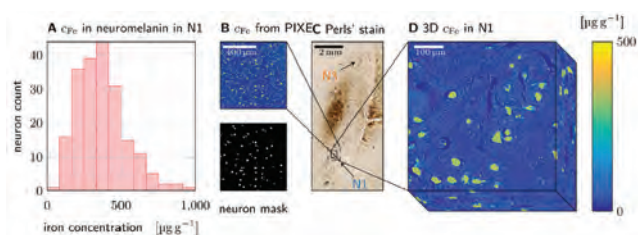

Figure 9: Quantitative iron histology of post mortem human-brain tissue with micro-PIXE. The research indicated a path to early markers for Parkinson's disease (From Brammerloh et al., Neuroimage 2021).

We carried out the project *Impact of the Brežice Hydroelectric Power Plant on the NPP Krško and the Environmental Impact Report for the extension of the NPP's operating life*. After the construction of the Brežice Hydroelectric Power Plant (HPP), new hydraulic conditions in the Sava River have emerged, which are not well known to us. The changes in the flow regime of the Sava River after the construction of the Brežice HPP are indicated by visual observations of the local population and by the evaluation of measured tritium activity concentrations at sampling stations in the flow storage of the Brežice HPP, above the dam of the Brežice HPP and in Brežice. It is noted that the dilution ratio has changed in Brežice, but is unknown at the other locations. According to the technical specification *Dose calculation and dilution modelling of run-of-river Brežice hydro plant accumulation No. TO. RZ-5/2020*, a numerical program will be developed to assess the population effects based on the evaluation of the dilution in the flow-through storage of the Brežice HPP using the tested PCFLOW3D model. An experimental study for the tracking of tritium levels in the Sava River downstream of the NPP was also proposed as one of the tasks of the project, and will be used for comparison between theoretical predictions of tritium activity concentrations in the Sava River and the measured values.

We undertook activities as a part of the project Implementation of a programme for systematic surveillance of the working environment in activities with materials containing naturally occurring radionuclides for 2021. The purpose of the project was to define and specify a programme to ensure the protection of workers and members of the public from an increased radiation exposure due to natural sources of radiation in areas and during activities with an increased risk of radiation from these sources. Handling and working with materials after thermal treatment (resulting from the processing of naturally occurring radioactive material) must not result in an excessive exposure of workers, considering external and internal irradiation (inhalation of dust particles). Due to the natural radioactivity of the materials, it should be borne in mind that the total effective dose to the worker is determined by the dose contributed by the gamma emitters Ra-226, Th-232 and K-40 and the effective dose absorbed in the lung tissue due to the uptake of the alpha emitting radon decay products Rn-222. When materials contain elevated specific activities of naturally occurring radionuclides, the ambient dose equivalent rate in the air inside the monitored facility is consequently increased. If the risk to workers' health from ionising radiation is to be reduced, it is necessary to control and place certain restrictions on the use of raw materials that might contain elevated concentrations of radionuclides. In addition, it is necessary to monitor these materials at all times and in good quality, and to prevent them from exceeding the limit values.

In this project we have focused on the working environment in activities producing thermal insulation and waterproofing end products (FRAGMAT TIM, d.o.o, Laško, ISOMAT, d.o.o Mežica) and in companies producing or using geothermal energy (Mavrica kindergarten, Brežice, and Ocean Orchids d.o.o, Dobrovnik). The level of radioactivity was estimated from the measurements of the ambient dose rate equivalent, spectrometric analyses of incoming raw materials, finished products and air by high-resolution gamma spectrometry, and measurements of indoor radon concentrations.

INTERNATIONAL PROJECTS

1. EMPIR; Preparedness - Metrology for Mobile Detection of Ionising Radiation Following a Nuclear or Radiological Incident
   Dr. Toni Petrovič
   Euramet E.v.
2. EMPIR - 17RPT01 DOSEtrace; Research Capabilities for Radiation Protection Dosimeters
   Denis Glavič Cindro, M. Sc.
   Euramet E.v.
3. EMPIR - supportBSS; Support for a European Metrology Network on Reliable Radiation Protection Regulation
   Denis Glavič Cindro, M. Sc.
   Euramet E.v.
4. EMPIR; AEROMET II; Advanced Aerosol Metrology for Atmospheric Science and Air Quality
   Asst. Prof. Klemen Bučar
   Euramet E.v.
5. Enhancing Nuclear Analytical Techniques to Meet the Needs of Forensic Sciences; Forensics with Nuclear Methods: Art and Food Forgery, Drugs in Hair
   Prof. Primož Pelicon
   IAEA - International Atomic Energy Agency
6. COST CA18130; European Network for Chemical Elemental Analysis by Total Reflection X-Ray Fluorescence
   Dr. Marijan Nečemer
   Cost Association Aisbl
7. COST CA18222; Attosecond Chemistry
   Asst. Prof. Andrej Mihelič
   Cost Association Aisbl
8. COST CA18212; Molecular Dynamics in the GAS Phase

Prof. Matjaž Žitnik
Cost Association Aisbl

9. COST CA16117; Chemical Elements as Tracers of the Evolution of the Cosmos
   Prof. Matej Lipoglavšek
   Cost Association Aisbl
10. TC Regional Project RER/7/014: Improving Environmental Monitoring and Assessment for Radiation Protection in the Region
    Asst. Prof. Benjamin Zorko
    IAEA - International Atomic Energy Agency
11. Experiments and Modelling of In Situ Uptake, Transport and Release Studies of Hydrogen Isotopes in Irradiated Tungsten; Hydrogen Permeation in Fusion-Relevant Materials
    Asst. Prof. Sabina Markelj
    IAEA - International Atomic Energy Agency
12. Detection of Hydrogen Isotopes by NRA, Cross Sections and Best Practices; Development and Application of Ion Beam Techniques for Materials Irradiation and Characterization Relevant to Fusion Technology
    Asst. Prof. Sabina Markelj
    IAEA - International Atomic Energy Agency
13. H2020 - TRANSAT; TRANSversal Actions for Tritium
    Asst. Prof. Sabina Markelj
    European Commission
14. H2020 - RADIATE; Research and Development with Ion beams - Advancing Technology in Europe
    Prof. Matjaž Kavčič
    European Commission
15. H2020 - CleanHME; Clean Energy from Hydrogen-Metal Systems
    Prof. Matej Lipoglavšek
    European Commission

16. H2020 - HITRIplus; Heavy Ion Therapy Research Integration
    Asst. Prof. Matjaž Vencelj
    European Commission
17. H2020 - EUROfusion; Plasma Facing Components-1-IPH-FU, EUROfusion
    Asst. Prof. Sabina Markelj
    European Commission
18. Study of Weak Charge Distributions with Precision Parity-Violating Measurements
    Asst. Prof. Miha Mihovilovič
    Slovenian Research Agency
19. Electrochemical Reactions in Organic-Metal Batteries Studied by X-Ray Raman Spectroscopy
    Prof. Matjaž Kavčič
    Slovenian Research Agency
20. Investigation of Helium Retention in Plasma Facing Materials Using Advanced Analytical Methods
    Asst. Prof. Sabina Markelj
    Slovenian Research Agency
21. HE - EUROfusion; WP07: ENR-DeHydroc-1,2,3_HE-FU
    Asst. Prof. Sabina Markelj
    European Commission
22. HE - EUROfusion; WP21: PRD-1,2_HE-FU
    Asst. Prof. Sabina Markelj
    European Commission
23. HE - EUROfusion; WP05: PWIE-1,2,3_HE-FU
    Asst. Prof. Sabina Markelj
    European Commission
24. HE - EUROfusion; WP24: TRED_HE-FU, EDU_HE-FU
    Prof. Primož Pelicon
    European Commission

RESEARCH PROGRAMMES

1. Archaeological and Archaeometric Research of Portable Archaeological Heritage
   Dr. Eva Menart
2. Object and Prestige; taste, status, power (Researches of the material culture in Slovenia)
   Dr. Marijan Nečemer
3. Parallel and Distributed Systems
   Prof. Roman Trobec
4. Structure of hadronic systems
   Prof. Simon Širca
5. Studies of atoms, molecules and structures by photons and particles
   Prof. Matjaž Žitnik
6. Fusion technologies
   Asst. Prof. Sabina Markelj

R & D GRANTS AND CONTRACTS

1. Ionom of crop plants for safe and quality food production
   Prof. Katarina Vogel-Mikuš
2. Structured light as a tool for triggering and probing new states of matter
   Prof. Matjaž Žitnik
3. Alternative approaches to assuring guality and security of buckwheat grain microbiome
   Prof. Primož Pelicon
4. Lessons from nutrient-use-efficient plants to benefit dietary mineral intake
   Prof. Primož Pelicon

5. Molecular imaging inside the cell
   Prof. Primož Pelicon
6. Catalysis of Nuclear Reactions by Electrons
   Prof. Matej Lipoglavšek
7. Molecular Imaging Inside the Cell
   Prof. Primož Pelicon
8. Spatial localization of elements and metabolits in plants
   Prof. Katarina Vogel-Mikuš
9. Novel proxies of the Holocene climate variability in stalagmites in Slovenia
   Prof. Primož Pelicon
10. Developing tender X - ray spectroscopy probes to tackle problems in materials science and ultrafast science
    Prof. Matjaž Kavčič
11. Detection of defects and hydrogen by ion beam analysis in channelling mode for fusion
    Asst. Prof. Sabina Markelj
12. Localy grown buckwheat grain for production of high quality food products
    Prof. Primož Pelicon
13. Innovative ECO plasma seed treatment (for sowing and for human and animal diet/nutrition)
    Prof. Primož Pelicon
    Ministry of Education, Science and Sport
14. Ecology laboratory with mobile unit
    Prof. Matej Lipoglavšek
    Ministry of Defence
15. Monitoring of radioactivity in drinking water for years 2020 and 2021 (lot 2)
    Asst. Prof. Benjamin Zorko
    Ministry of Health
16. Calibrations
    Boštjan Črnič
17. Different Analyses; Reference Materials
    Dr. Jasmina Kožar Logar
18. CROSSING - Crossing Borders and Scales - An Interdisciplinary Approach
    Prof. Primož Pelicon
    Helmholtz-Zentrum Dresden-Rossendorf E.v.
19. C-14 Measurements
    Dr. Romana Krištof

NEW CONTRACTS

1. Measurements of gaseous effluents, specific analysis of H-3 and C-14 in year 2021
   Asst. Prof. Benjamin Zorko
   Krško Nuclear Power Plant
2. Maintaining emergency preparedness and response by ELME (2020-2023)
   Asst. Prof. Benjamin Zorko
   Krško Nuclear Power Plant
3. Environmental radioactivity monitoring in the vicinity of the Krško Nuclear Power Plant (drinking water, air, food, Sava River, precipitation, soil and external radiation in the environment with the dose assessment)
   Asst. Prof. Benjamin Zorko
   Krško Nuclear Power Plant
4. Environmental radioactivity monitoring in the vicinity of the Krško Nuclear Power Plant in connection with Hydro Power Plant Brežice for the years 2020 and 2021
   Asst. Prof. Benjamin Zorko
   Krško Nuclear Power Plant
5. Report on the environmental impact assessment of the Brežice hydroelectric power plant and the impact on the operational lifetime extension of the Krško NPP
   Asst. Prof. Benjamin Zorko
   Krško Nuclear Power Plant

VISITORS FROM ABROAD

1. Bo Hu, Czech University of Life Sciences Prague, Prague, Czech Republic, 1 November – 31 December 2021
2. Despina Daniella Magueranu in dr Roxana Nicoleta Bugoi, Institute of Archaeology "Vasile Pârvan", Bucharest, Romania, 13–17 December 2021

STAFF

Researchers
1. Prof. Iztok Arčon*
2. Asst. Prof. Klemen Bučar
3. Prof. Dean Cvetko*
4. Denis Glavič Cindro, M. Sc.
5. Dr. Darko Hanžel
6. Prof. Matjaž Kavčič
7. Dr. Jasmina Kožar Logar
8. Dr. Romana Krištof*
9. Prof. Matej Lipoglavšek
10. Asst. Prof. Sabina Markelj
11. Asst. Prof. Andrej Mihelič
12. Asst. Prof. Miha Mihovilovič
13. Dr. Marijan Nečemer
14. **Prof. Primož Pelicon, Head**
15. Dr. Toni Petrovič*
16. Dr. Paula Pongrac*
17. Prof. Simon Širca*
18. Dr. Primož Vavpetič
19. Asst. Prof. Matjaž Vencelj

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ORIGINAL ARTICLE

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41. I. Mardor *et al.* (56 authors), "Mass measurements of As, Se, and Br nuclei, and their implication on the proton-neutron interaction strength toward the N = Z line", *Physical review. C*, 2021, **103**, 3, 034319.

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4. Toni Petrovič, "Radioaktivnost v usedih", In: *Ovrednotenje meritev radioaktivnosti v reki Savi, pitni vodi, padavinah, zraku, zemlji in hrani v okolici NEK in po Sloveniji*, Institut "Jožef Stefan", 2021, 106-37-106-48.

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University, Higher Education or Higher Vocational Education Textbook

1. Simon Širca, *Verjetnost v fiziki*, Fakulteta za matematiko in fiziko, 2021.

Theses and Mentoring

1. Eyakifama Hazou, *Etude par spectrométrie gamma de l'impact radiologique des échantillons environnementaux provenant des sites d'exploitation du phosphate des localités de Hahotoé Kpogamé Kpémé (Sud Togo) sur le public:* doctoral dissertation, Ljubljana, 2021 (mentors Komi Paalamwé Tchakpele, Benjamin Zorko).
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3. Matic Pečovnik, *The influence of hydrogen isotopes on the behaviour of crystal lattice defects in tungsten:* doctoral dissertation, Ljubljana, 2021 (mentor Sabina Markelj).
4. Isabela Tišma, *Nuclear reactions relevant to Big-Bang nucleosynthesis:* doctoral dissertation, Ljubljana, 2021 (mentor Matej Lipoglavšek; co-mentor Miha Mihovilovič).

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.

For several years we have been working on the topic of growth defects in hard coatings. Being interesting from the application side, yet relatively poorly explained in the literature, these activities have a high impact. The appearance of growth defects in coatings prepared by physical vapor deposition (PVD) has been known for a long time, but knowledge is limited about their influence on the coating behavior in real working conditions.

In one of our research projects we concentrated on the question of the initial stages of hard coating oxidation. We selected the standard TiAlN coating and exposed it to 600–850 °C, which is in the range of temperature peaks at the cutting edge during machining processes. We analyzed the surface after oxidation and performed micrometer-scale cross-sections of selected areas using the focused-ion-beam technique (FIB). A thin Al_2O_3 oxide layer formed on the surface, which generally protects against further oxidation, thus one could tentatively consider that the sample has not experienced any meaningful damage. Nevertheless, at the local level the conditions are much different.

We proved this at the positions of pinholes; they are no wider than a few hundred nanometres, but extending down to the substrate, they act as shortcuts for oxygen diffusion. Nodular defects play a similar role as they start to grow at the substrate, and they border the undamaged part of the coating by a heavily porous surface. We analyzed several growth defects and characterized to what extend they act as starting points for oxidation.

A typical topography analysis is often limited to surface roughness as a consequence of the substrate roughness and thin-film growth. In order to obtain a concise overview of the mechanisms contributing to the surface topography we performed a systematic analysis of all the factors that contribute to the final result. We evaluated the contributions of the substrate material, surface mechanical treatment, ion etching and thin-film growth. This was performed for several different methods of ion etching and deposition, and we published the results in a review paper.

In our department we have been studying plasma processes in magnetron discharges for several years. We analyze the processes using different plasma diagnostics techniques, such as mass spectrometer, optical emission spectroscopy, high-speed camera, electrical probes and others. Using these techniques in the previous year, we studied plasma inhomogeneities (so-called ionization zones) that appear in magnetron discharges. We concentrated specifically on plasma studies of high-power impulse magnetron sputtering (HiPIMS) and DC regimes. A comparison of the plasma in these two regimes showed several differences in plasma inhomogeneity properties. In the DC regime plasma forms predominantly periodic patterns while the ionization zones have an arrow-like form. In the pulse regime, on the other hand, the plasma patterns are less periodic, the zones are shorter and in triangular forms. The dynamics of ionization zones is different too. In the DC regime the zones move in the direction opposite to the electron movement, while in the HiPIMS regime they move in the same direction as the electrons.

We have been active in fusion research within the EUROfusion consortium, where we study the surfaces of materials at the reactor first wall, which is in direct contact with the hot plasma. Last year we utilized the focused-ion-beam technique to analyze the changes in morphology and composition in tungsten tiles that had been induced by strong discharge arcing between the plasma and the wall of the ASDEX Upgrade fusion reactor (Garching,

Head:
Prof. Miha Čekada
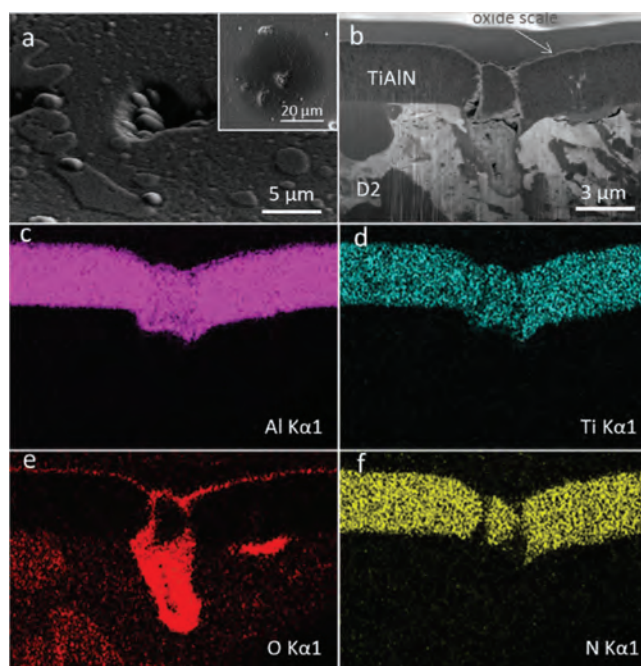
Figure 1: A pinhole in the TiAlN coating after exposure to 800 °C. At the image of the surface (a) the pinhole opening is barely visible, while in a cross-section (b) there are two clear channels, extending across the whole coating towards the substrate. Maps of individual elements are shown in figures (c–e) where a high oxygen concentration is visible in the substrate, just below both channels.

Germany). Using X-ray photoelectron spectroscopy (XPS) we also analyzed several beryllium thin films with different deuterium concentrations.

In the scope of an informal collaboration with Montanuniversität Leoben (Austria) and the University of California, Berkeley (USA), we measured the trend of fracture toughness of the CrAlN and CrAlSiN coatings up to a temperature of 700 °C in 100 °C steps. Using an in-situ nanomechanical tester we loaded each microlever up to the point of breaking. By applying the finite-element method we evaluated the geometrical constraints and determined the dimensionless parameter necessary for a fracture-toughness calculation. The high-temperature fracture toughness was linked to the acquired results for high-temperature hardness of the material, and high-temperature measurements of the friction coefficient and wear.
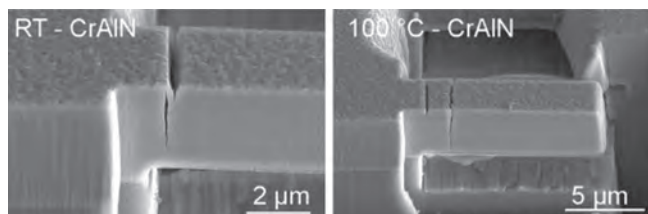

Figure 2: Microlevers prepared from a CrAlN coating after a loading test to determine the fracture toughness

Our research is often directed towards applications of the coatings for specific machining processes. We put a lot of effort in evaluating the coatings deposited in industrial deposition systems, where our primary interest is the influence of process parameters on coating properties. In the previous year we concentrated on precise measurements of property dependence on vertical position for typical shank tools. We have been collaborating with the Mechanical Engineering Faculty, University of Ljubljana, in the field of hard-coating lifetime in applications using liquid CO_2 as the cooling medium in semi-industrial conditions. We evaluated the wear resistance of several different coatings, with an emphasis on TiAlSiN and TiAlN. In addition to testing in semi-industrial conditions we also constructed a set-up in a laboratory environment at a tribometer, which will be a topic of research in the coming year. We had an additional project with the Mechanical Engineering Faculty in the topic of developing TiO_x optoacoustic lenses; we confirmed comparable tribological properties as the fullerene-like MoS_2, synthesized using a new, faster method.

We evaluate the applicability of our coatings for specific applications with foreign partners too. We need to stress the collaboration with the University of Novi Sad (Serbia) where we evaluated the influence of nanolayer coatings on the reduction of melt adhesion on tools for aluminum die casting. The paper was published in SVC Bulletin, which is the key technologically oriented journal in the topic of protective coatings and well known in industrial circles. We should also mention the research with Warsaw Technical University on the topic of protecting cutting inserts for wood machining using nanolayer AlTiN coatings and amorphous carbon-based coatings. At the level of basic research, we study the magnetic properties of nanoparticles with different shapes, prepared by hydrothermal analysis; this is performed in collaboration with the Vinča Institute of Nuclear Sciences from Serbia. We are also interested in the magnetic properties of nanoparticles in connection with therapeutic applications for drug delivery.

The department intensively collaborates with Slovenian industry. The companies ask for support in the case of issues related to surfaces and thin films. This can include R&D projects, advanced analytics or failure analysis. In the previous year we performed such tasks for the following companies: Cetis, Difa, Domel, Hella, Iskra mehanizmi, Jordan, Kern, Kolektor, Kovinos, Le-tehnika and Phos. We also offer the companies the service of depositing hard coatings on their tools, which we perform within the Hard Coatings Center, which operates within the department. There are more than a hundred partners annually, which includes both large companies (e.g., Kolektor, Mahle, Hidria) as well as numerous small workshops.

Figure 3: Case of a test batch construction in the industrial deposition chamber; we applied polished high-speed steel rods for the continuous vertical evaluation of the coating properties.

Some outstanding publications in the past year

1. P. Panjan, A. Drnovšek, N. Mahne, M. Čekada, M. Panjan, Surface topography of PVD hard coatings. *Coatings*, ISSN 2079-6412, 2021, vol. 11, no. 11, pp. 1–31

2. M. Čekada, P. Panjan, A. Drnovšek, M. Drobnič, Increase of coating thickness on sharp edges, deposited by cathodic arc evaporation. *Surface & coatings technology*, ISSN 0257-8972, 2021, vol. 405, pp. 126691-1–126691-8

3. A. Drnovšek, H. T. Vo, M. R. de Figueiredo, S. Kolozsvari, P. Hosemann, R. Franz, High temperature fracture toughness of single-layer CrAlN and CrAlSiN hard coatings, *Surface & coatings technology*, ISSN 0257-8972, 2021, vol. 409, pp. 126909-1–126909-7

INTERNATIONAL PROJECTS

1. HE - EUROfusion; WP05: PWIE-1,2,3_HE-FU
   Dr. Matjaž Panjan
   European Commission

RESEARCH PROGRAMME

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

R & D GRANTS AND CONTRACTS

1. Initial stages in surface functionalization of polymers by plasma radicals
   Uroš Stele

2. Self-organization of plasma in magnetron sputtering discharges
   Dr. Matjaž Panjan
3. Controllable broadband electromagnetic-radiation shielding
   Dr. Matjaž Panjan
4. Carbon nanowalls for future supercapacitors
   Prof. Miha Čekada
5. Selected area functionalization of polymeric components by gaseous plasma
   Prof. Miha Čekada
6. Waterborne virus inactivation efficiency of a prototype device combining non-equilibrium plasma and hydrodynamic cavitation
   Prof. Miha Čekada
7. Innovative ECO plasma seed treatment (for sowing and for human and animal diet/nutrition
   Prof. Miha Čekada
   Ministry of Education, Science and Sport
8. Deposition of hard coatings
   Prof. Miha Čekada

VISITORS FROM ABROAD

1. Dubravka Milovanović, Biljana Gaković, Institute of General and Physical Chemistry, Belgrade, Serbia, 12.–16. 7. 2021
2. Marco Beltrami, University of Trieste, Trieste, Italy, 20. 7. 2021
3. Marco Beltrami, University of Trieste, Trieste, Italy, 28.–29. 7. 2021
4. Marin Tadić, Vinča nuclear institute, Belgrade, Serbia, 20. 9.–1. 10. 2021
5. Pal Terek, Vladimir Terek, University of Novi Sad, Novi Sad, Serbia, 30. 9.–12. 10. 2021

STAFF

Researchers
1. Prof. Miha Čekada, Head
2. Dr. Aljaž Drnovšek
3. Dr. Matjaž Panjan
4. *Dr. Peter Panjan, retired 5. 10. 2021*
Postgraduates
5. Matej Drobnič, B. Sc.
6. Žan Gostenčnik, B. Sc.
7. Nastja Mahne, B. Sc.

Technical officer
8. Uroš Stele, B. Sc.
Technical and administrative staff
9. Jožko Fišer
10. Damjan Matelič
11. Andrej Mohar
12. Tomaž Sirnik
13. Tadej Stele

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4. Peter Panjan, Aljaž Drnovšek, Nastja Mahne, Miha Čekada, Matjaž Panjan, "Surface topography of PVD hard coatings", *Coatings*, 2021, **11**, 11, 1387.
5. Biljana Gaković, Pavel A. Danilov, Sergey I. Kudryashov, Dragan Milovanović, Aleksandra Radulović, Peter Panjan, Andrey A. Ionin, "The morphological and compositional changes of bimetallic Ti/Al thin film induced by ultra-short laser pulses", *The European physical journal. D., Atomic, molecular, optical and plasma physics.*, 2021, **75**, 11, 288.
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10. Dragan Kukuruzović, Pal Terek, Lazar Kovačević, Branko Škorić, Aleksandar Miletić, Peter Panjan, Miha Čekada, "Investigation of CrAlN coatings soldering resistance for high pressure die casting tools", In: *SVC Bulletin*, Fall/Winter 2021, 90-96.
11. Nastja Mahne, Matjaž Panjan, "Obstreljevanje trdnih snovi z ioni. II., Simulacije razprševanja atomov", *Vakuumist: glasilo Društva za vakuumsko tehniko Slovenije*, 2021, **41**, 1/2, 4-11.

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2. Daniele Vella, Blaž Tašič Muc, Nejc Lukač, Matjaž Kos, Aljaž Drnovšek, Matija Jezeršek, "Microstructured optoacoustic lens of black-TiO_x for focused ultrasound and confined cavitation bubbles", In: *European Conference on Biomedical Optics 2021 (ECBO), 20-24 June 2021, Munich, Germany*, Proceedings, OSA, 2021, EM1A.32.

DEPARTMENT OF SURFACE ENGINEERING AND OPTOELECTRONICS F-4

The Department of Surface Engineering conducts interdisciplinary research on designing the surface properties of various materials. We use advanced techniques for surface and thin-film characterization, in particular with our XPS, AES, SIMS and AFM instruments. The scientific activities are focused on surfaces and coatings, gaseous discharges, thermodynamically non-equilibrium plasma and the interaction of reactive plasma species with organic and inorganic materials. Patent applications protect innovative solutions for industry, medicine, biotechnology and agriculture.

JSI is a project partner in the H2020-CSA Athena project (https://www.athenaequality.eu/), which aims to remove barriers to the recruitment, retention and career progression of female researchers, lowering gender imbalances in decision-making processes and generating a cultural change needed to avoid gender bias and discriminatory practices through the implementation of Gender Equality Plans (GEPs). To ensure systemic institutional change, the project plans to conduct an assessment of procedures and practices already in place in partner organizations, together with an analysis of the national legislation and policy frameworks. In parallel, it will put in place a participatory process aimed, on one hand, to understand the needs and the preferences of the stakeholders and, on the other, to train them about selected topics related to gender. As a final result, each partner organization will draft and implement its specific GEP.

At the Jožef Stefan Institute, the Athena activities are carried out by 9 research departments and the Director's office. The Department of Surface Engineering participated in the identification of existing gender bias at the organisational level as well as in the assessment of existing national provisions. We were involved in gathering information on gender bias at the JSI by conducting story-telling interviews and discussions in different focus groups (managers, researchers, administration, young researchers and members of the Gender Equality Plan Implementation (GEPI)). Our representative is also a member of the GEPI committee, which is the leading body at the organisation for the preparation and implementation of the GEP. In this role, all the GEPI members have to pass the compulsory education courses given by the coordinator, which will be further disseminated at the JSI. In addition, our department is active in dissemination and communication activities. The news about the project can be found at JSI website (https://www.ijs.si/ijsw/EnakeMoznosti) as well as at Athena website (https://www.athenaequality.eu/).

The major activities of the Department F4 remain scientific research and the development of technological solutions useful for applications in mass production. The surface functionalization of organic materials remains a hot topic of interdisciplinary science, where plasma physics meets surface chemistry, biology, and agriculture. Despite a tremendous commercial potential, the exact mechanisms of surface functionalization upon treatment with molecular fragments on the atomic scale remain unexploited due to the complexity of the interaction. A lack of reliable theories is partially compensated by precisely designed experiments. Gaseous plasma is a source of various radicals and charged particles as well as radiation across a broad range from infrared to vacuum ultraviolet, so it is far too complex for a detailed scientific investigation. The surface functionalization is often accomplished by neutral species such as atoms. We designed an experimental setup useful for the adjustment of the density of neutral oxygen atoms in the ground electronic state in the range from approximately 10^{17} to 10^{22} m^{-3}. The system powered by a radio-frequency (RF) electrodeless discharge is optimized for studying the surface kinetics versus the doses of O atoms. We used polystyrene as a model polymer of a well-defined structure. This polymer has recently been tackled also by theoreticians who identified over ten binding sites of different binding energies even for pristine polystyrene, more for partially oxidized material. We studied the evolution of surface functional groups versus the dose of atoms starting at the dose as small as 10^{19} m^{-2} and found an excellent agreement with the theoretical predictions. The evolution of the functional groups is shown in Figure 1. Considering the peculiarities of XPS, we can conclude that

Head (since 1. 12. 2021):
Prof. Alenka Vesel

Head (until 30. 11. 2021):
Prof. Miran Mozetič

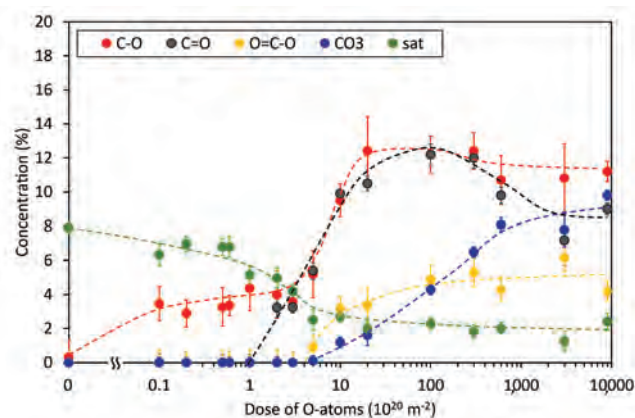**We confirmed the recent theory of the functionalization of aromatic polyolefins.**

Figure 1: *The concentration of surface-functional groups versus the dose of O atoms. Reproduced from [1].*

the formation of hydroxyl groups on the pristine polystyrene is a highly probable reaction. The surface saturation with hydroxyl groups is accomplished already at the dose of approximately 10^{19} m^{-2}. Once the surface is saturated with hydroxyl groups, the further treatment causes gradual destruction of the phenyl ring and thus the formation of the surface sites capable of the irreversible binding of oxygen in other functional groups. The concentration of hydroxyl groups starts increasing above the saturation level after receiving the dose of 3×10^{20} m^{-2}, which is explained by the etching of the polymer and thus assuming a rich morphology on the scale measured in nanometres. Such a rich morphology causes the virtual surface concentration of oxygen as probed by XPS well above the theoretical limit. Details about the surface kinetics were published in the journal ranked #1 in the scientific niche of "material science, coatings & films" [1].

The functionalization of polymers with polar, oxygen-containing functional groups is beneficial for increasing the surface wettability of all materials. While polystyrene is perhaps the most useful material for studying the evolution of the surface functional groups, the largest technological challenge is the functionalization of biological materials. The kinetics has not been tackled by any group worldwide, probably because of the complexity of the surface interactions. We treated corn seeds in oxygen plasma sustained by inductively coupled RF discharge at various pressures. The absorption of RF power by charged particles in gaseous plasma depends enormously on the gas pressure and forward discharge power because the plasma is sustained in either the E or H mode. The fluxes of some reactive plasma species change by several orders of magnitude at the transition between the modes, so the surface wettability obtained at a certain plasma treatment time depends enormously on the discharge mode. Still, according to the discussion in the previous paragraph, the decisive parameter governing the surface wettability should be the dose of O atoms. We plotted the surface wettability as determined by the sessile drop method versus the doses and actually observed the curve shown in Figure 2. Therefore, we clearly showed that irrespective of the treatment time, gas pressure, or discharge power, the surface wettability follows the general curve. Such an observation has not been reported in scientific literature, so our paper, published in the prominent journal in the niche of agriculture, can be regarded as a pioneering work in the niche of plasma agriculture.
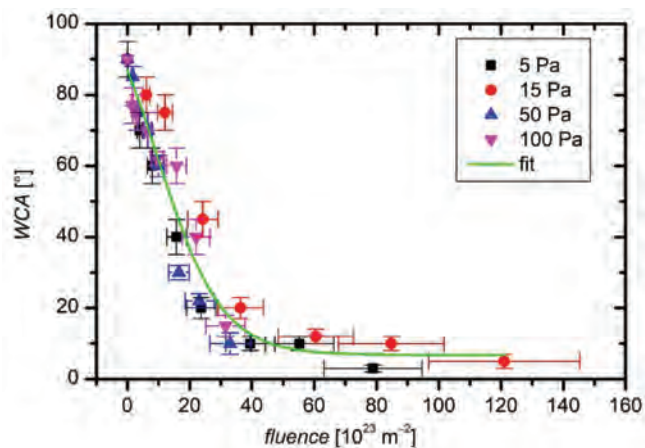

Figure 2: The surface wettability of corn seeds versus the doses of oxygen atoms. Reproduced from [2].

The team developed methods for the rapid inactivation of viruses on respiratory masks.
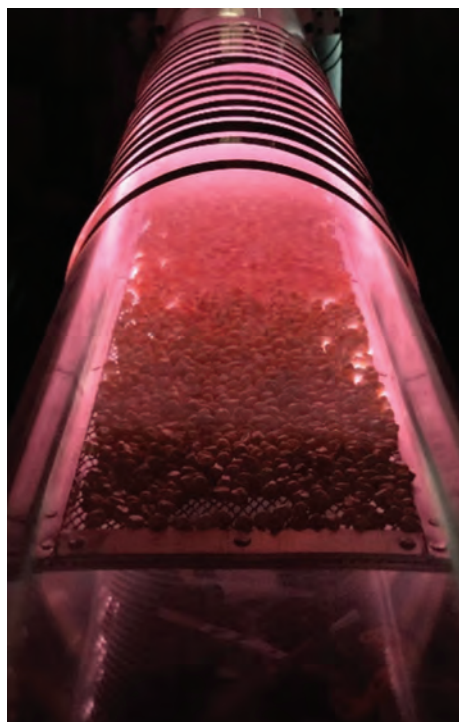

Figure 3: Low-pressure plasma is useful for the decontamination and hydrophilization of seeds before sowing. Reproduced from [2].

An appropriate wettability of seeds is useful for immediate water uptake and thus germination of the seeds, even in harsh conditions. The beneficial effect of plasma treatment has been reported by all partners of the COST action CA19110 "Plasma Applications for Smart and Sustainable Agriculture" https://plagri.eu/, where the member of our team, dr. Gregor Primc, serves as the Science Communications Manager. We performed a comprehensive literature survey [3] and found that very few groups worldwide reported on the mass application of the plasma technology and field experiments, so the plasma treatments are still at low technological readiness levels (TRLs). Our group successfully accomplished a large project on upscaling the TRL from 3 to 6. The project entitled "Plasma seed treatment" gathered research groups from 6 partners to develop a prototype of an industrial line for the treatment of about 1 ton of seeds per hour. The coordinator of this project, which was co-funded by European structural funds and the Slovenian Ministry of Agriculture, was the largest Slovenian company for trading seeds, Interkorn Ltd, whose Director is dr. Peter Gselman, and the scientific coordinator was dr. Nina Recek from Department F4. In fact, our department was the only public research organization involved in this project. Other partners were responsible for the construction, automatization, and verification of the prototype lines. We constructed several plasma reactors for the treatment of seeds, and one is shown in Figure 3. The consortium filed several patent applications, which will be published in the future, so we cannot disclose the methods of the invention. This was one of the largest projects involving both industrial research and experimental development in the history of the Jozef Stefan Institute. The research on plasma agriculture was performed by members of several research departments of our institute and the group at the Biotechnical Faculty, University of Ljubljana. The group of Dr. Katarina Vogel-Mikuš revealed the biological aspects of the plasma techniques and supervised Ph.D. students J. Mravlje and P. Starič [4], who will enlighten complex mechanisms of the biological response to non-equilibrium gaseous plasma.

The major income of the Department F4 comes from applied research projects that are co-funded by the Slovenian Research Agency (ARRS) and a company that is interested in the com-

mercialization of scientific knowledge. A fruitful collaboration has been established with the company Elvez Ltd., which uses several large plasma reactors in mass production. The typical volume of a plasma reactor is several cubic meters. Currently, it is believed that uniform plasma cannot be sustained with useful parameters in such large industrial reactors for numerous reasons, including the final penetration depth of electromagnetic radia-tion from the RF-powered electrodes, surface loss of radicals and charged particles, gas-phase oligomerization of the molecular fragments and the formation of dusty plasma. There has been a lack of appropriate methods for measuring the deposition rate of coatings prepared by plasma-enhanced chemical vapor deposition (PECVD). In collaboration with experts from the Laboratory for Electro-Optics and Sensor Systems, University of Maribor, we developed miniature sensors for real-time measurements of the deposition in PECVD systems. The group led by dr. Denis Đonlagić verified the laboratory prototypes of these sensors, and we performed systematic measurements at the premises of Elvez Ltd. company. We used a cylindrical plasma reactor with a diameter and height over 2 m and distributed the sensors at various positions, as shown in the inset of Figure 4. We measured the thickness of the protective coating deposited by the plasma polymerization technique. The lines in Figure 4 exhibit almost optimal linearity due to the careful selection of the adjustable discharge parameters. The slopes of the lines in Figure 4 indicate deposition rates that can vary by an order of magnitude, depending on the position in the industrial reactor for PECVD of polymer-like hydrophobic coatings. Optimization of such industrial reactors is among our key technological challenges for the future [5].
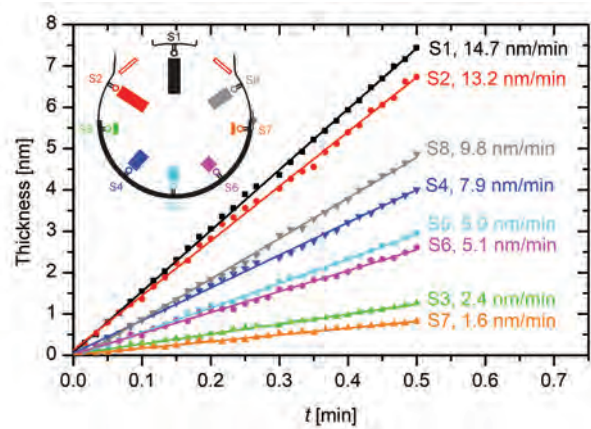

Figure 4: Schematic of the positions of miniature sensors (inset) and the thickness of the deposited films versus deposition time. Reproduced from [5].

The spread of the SARS-CoV-2 virus influenced our scientific and tech-nological activities significantly. We summarized the results on the virus infectivity of various materials and found insignificant differences in survival rates on different materials. Our research group proposed several methods for treating respiratory masks and prepared a patent application on the most promising and feasible technique based on plasma technology (Figure 5 and 6). Meanwhile, we also studied a process for the recycling of single-use per-sonal protective masks. We developed an efficient sterilization procedure. In collaboration with other departments at the Jozef Stefan Institute, we studied the sterilization options using gamma rays and high-energy electrons as well as the relationship between the irradiation, particle removal efficiency, and surface potential on the respirators [6]. The principal investigator in our group was dr. Janez Kovač. He characterized the chemical composition and the changes in static charge for polypropylene fibers from the filter piece of typical FFP3 masks after different types of ionizing sterilization. With our sensitive, non-contact measurements of the surface potential, we found that sterilization with X-rays and e-beam leads to complete removal of the surface charge, which is needed for electrostatic interaction for filtering particles of the virus size. In the next step after sterilization, we successfully recharged the sterilized filter surface to its initial potential. Sterilization and recharg-ing resulted in a complete regeneration of filtering facepiece respirators for protection against Covid-19.

Figure 5: Our plasma technologies make it possible to alter the surface energy of materials for masks against virus infections.

The F4 department performs basic research within two core-funding research programmes. The activities reported in the text above were per-formed within the core funding "Thin Film Structures and Plasma Surface Engineering," which is led by dr. Miran Mozetič. Another core funding is for "Fusion Technologies," and the principal investigator in our department is dr. Rok Zaplotnik. Our fusion-oriented scientific activities were focused on the scientific and technological challenges for fusion reactors beyond ITER. The

Figure 6: Image shows the dosing of the water drop to the surface of the untreated mask. If the mask is treated the water drop is absorbed.

divertor, which is positioned at the bottom of the vacuum vessel of a fusion reactor, controls the exhaust of waste gases (in particular helium) and impurities from the reactor and is subjected to the highest surface heat loads of the tokamak. In ITER, the diverter will be coated with tungsten, but this material has several drawbacks, so tungsten might be omitted in fusion reactors beyond ITER. For example, the next-generation machine is the demonstration power plant DEMO. The final design of the divertor in DEMO is not yet determined. For DEMO and beyond, liquid

metal plasma-facing components are also being considered. Liquid tin is believed to be one of the candidates for a liquid metal divertor. Our study focused on hydrogen solubility and deuterium-atom retention in the liquid Sn. An immeasurably low concentration of deuterium was detected in pure tin, but we observed significant retension in the tin-oxide layer, which might be due to the formation of hydroxides. We reported the results of our systematic research in [7]. Apart from the conclusion that the retention of hydrogen isotopes in the liquid-tin divertor free from oxide is unlikely, we also provided a recipe for effectively reducing the tin-oxide layer.

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Awards and Appointments

1. Ita Junkar, Metka Benčina, Matic Resnik, Rok Zaplotnik: Best innovation with commercial potential award, Center for Technology Transfer and Innovation at the Jožef Stefan Institute, Novel surface finishing procedures for medical devices, especially vascular stents.

Patents granted

1. Ita Junkar, Rok Zaplotnik, Metka Benčina, Miran Mozetič, Method for treatment medical devices made from nickel-titanium (NiTi) alloys, EP3636294 (B1), European Patent Office, 17. 11. 2021.
2. Gregor Filipič, Kristina Eleršič, Darij Kreuh, Janez Kovač, Uroš Cvelbar, Miran Mozetič, A method of colouring titanium and titanium alloys, GB2530805 (B), Intellectual Property Office, 24. 11. 2021.

INTERNATIONAL PROJECTS

1. COST CA18113; Understanding and Exploiting the Impact of Low pH on Microorganisms
Dr. Martina Modic
Cost Association Aisbl
2. COST CA19110; Plasma Applications for Smart and Sustainable Agriculture
Asst. Prof. Gregor Primc
Cost Association Aisbl
3. COST CA20114 - PlasTHER; Therapeutical Action of Cold Atmospheric Plasmas
Asst. Prof. Ita Junkar
Cost Association Aisbl
4. H2020 - PEGASUS; Plasma Enabled and Graphene Allowed Synthesis of Unique nano Structures
Prof. Uroš Cvelbar
European Commission
5. H2020 - ATHENA; Implementing Gender Equality Plans to Unlock Research Potential of RPOs and RFOs in Europe
Asst. Prof. Ita Junkar
European Commission
6. H2020 - EUROfusion; Plasma Facing Components-1-IPH-FU, EUROfusion
Asst. Prof. Rok Zaplotnik
European Commission
7. H2020 - EUROfusion; JET Campaigns-JET1-FU
Dr. Aleksander Drenik
European Commission
8. H2020 - EUROfusion; WPPFC-PEX-FU, WPPFC-PEX-FU, EUROfusion
Asst. Prof. Rok Zaplotnik
European Commission
9. Catalytic Probes for Characterization of Hydrogen Plasma
Asst. Prof. Gregor Primc
Slovenian Research Agency
10. Control of Chemical Composition of Thin Films by High Resolution Mass Spectrometry

of Secondary Ions
Prof. Janez Kovač
Slovenian Research Agency
11. Advanced Catalysts based on Multilayered Vertically Oriented Graphene Nanostructures
Prof. Alenka Vesel
Slovenian Research Agency
12. Investigation of Helium Retention in Plasma Facing Materials Using Advanced Analytical Methods
Dr. Gregor Filipič
Slovenian Research Agency
13. Characterization of Oxygen Plasma Sustained with Powerful Gaseous Discharges
Prof. Miran Mozetič
Slovenian Research Agency
14. Low Temperature Plasma Diagnostics and its Applications for Seed Treatment
Prof. Miran Mozetič
Slovenian Research Agency
15. Functionalization of Ti-Based Surfaces Using Energy Beams and Plasma for Biomedical Applications
Asst. Prof. Gregor Primc
Slovenian Research Agency
16. Promising Eco-Sterilization of Pathogenic Fungi on Seeds Using Reactive Species in Gaseous Plasma
Prof. Miran Mozetič
Slovenian Research Agency

RESEARCH PROGRAMMES

1. Vacuum technique and materials for electronics
Dr. Vincenc Nemanič
2. Thin film structures and plasma surface engineering
Prof. Miran Mozetič
3. Fusion technologies
Asst. Prof. Rok Zaplotnik

R & D GRANTS AND CONTRACTS

1. Structural and surface properties of fibrous membranes for purification and chromatographic separation of biomacromolecules
Asst. Prof. Ita Junkar
2. Ecologically friendly in-situ synthesis of ZnO nanoparticles for the development of protective textiles
Asst. Prof. Gregor Primc
3. Initial stages in surface functionalization of polymers by plasma radicals
Prof. Janez Kovač
4. Alternative approaches to assuring guality and security of buckwheat grain microbiome
Prof. Miran Mozetič
5. Advanced surface finishing technologies for antibacterial properties of patient specific 3D printed implantable materials
Asst. Prof. Ita Junkar
6. Hybrid and Reengineered Nanocatalysts for New Purification Routes
Prof. Janez Kovač
7. Self-organization of plasma in magnetron sputtering discharges
Prof. Miran Mozetič
8. New startegies for fabrication of biomimetic vascular implants
Asst. Prof. Ita Junkar
9. Innovative procedures for advanced surface properties of medical stainless steel
Dr. Metka Benčina
10. Development of new, environment-friendly approaches for plant and human virus inactivation in waters
Asst. Prof. Gregor Primc
11. Innovative sensors for real-time monitoring of deposition rates in plasma-enhnced chemical vapour deposition (PECVD) systems
Asst. Prof. Rok Zaplotnik
12. Nanoparticle-reinforced new metal matrix composites manufactured by selective laser

melting for tooling industry
Prof. Miran Mozetič
13. A Novel High-strength Aluminium Alloy developed for Selective Laser Melting and Lightweight Applications
Prof. Miran Mozetič
14. Innovative configuration of inductively coupled gaseous plasma sources for up-scaling to industrial-size reactors
Prof. Miran Mozetič
15. Carbon nanowalls for future supercapacitors
Prof. Alenka Vesel
16. Selected area functionalization of polymeric components by gaseous plasma
Prof. Miran Mozetič
17. Innovative method for purification of wastewater
Asst. Prof. Gregor Primc
18. Development of safe multifunctional surfaces for catheters to combat biofilms (DemoCat)
Prof. Alenka Vesel
19. Waterborne virus inactivation efficiency of a prototype device combining non-equilibrium plasma and hydrodynamic cavitation
Asst. Prof. Rok Zaplotnik
20. Use of gaseous plasma for higher yields and lower use of antifungal agents in agriculture
Asst. Prof. Ita Junkar
21. Innovative ECO plasma seed treatment (for sowing and for human and animal diet/nutrition
Dr. Nina Recek
Ministry of Education, Science and Sport
22. Method for preparation of bacteriostatic surfaces on 3D printed medical implants
Dr. Matic Resnik
Ministry of Education, Science and Sport
23. Use of gaseous plasma for higher yields and lower use of antifungal agents in agriculture
Asst. Prof. Ita Junkar
Ministry of Agriculture, Forestry and Food
24. Income from Coowners of Invention for Reimbursement of Costs for IP Protection in the Case of EVT140_Mozetič_Carbon Nanowall
Prof. Miran Mozetič
Nagoya University
25. EVT770_Mozetič_CNW2_Reimbursement of the Costs for Patent; Income from Coowners of Invention for Reimbursement of Costs for IP Protection in the Case of EVT770_Mozetič_CNW2
Prof. Miran Mozetič
Nagoya University

NEW CONTRACTS

1. Innovative configuration of inductively coupled gaseous plasma sources for up-scaling to industrial-size reactors
Prof. Miran Mozetič
Vacutech vakuumske zehnologije in sistemi d. o. o.
2. Regulation of mutual relations between the Company and JSI in joint research and development („KET4CleanProduction")
Asst. Prof. Ita Junkar
Brinox Inženiring d. o. o.
3. Co-finanicing of L-project L2-1834 Carbon nanowalls for future supercapacitors
Prof. Alenka Vesel
Iskra, d. o. o.
4. Innovative sensors for real-time monitoring of deposition rates in plasma-enhanced chemical vapour deposition (PECVD) systems
Asst. Prof. Rok Zaplotnik
Iskra, d. o. o.
5. L-project co-financing: Innovative method for purification of wastewater
Asst. Prof. Gregor Primc
Induktio d. o. o.
6. L-project co-financing: Selected area functionalization of polymeric components by gaseous plasma
Prof. Miran Mozetič
Elvez, d. o. o.

STAFF

Researchers
1. *Dr. Aleksander Drenik, on leave since 01.03.16*
2. Asst. Prof. Ita Junkar
3. Prof. Janez Kovač
4. **Prof. Miran Mozetič, Head, until 30. 11. 2021**
5. Asst. Prof. Gregor Primc

6. **Prof. Alenka Vesel, Head, since 1. 12. 2021**
7. Asst. Prof. Rok Zaplotnik
Postdoctoral associates
8. Dr. Metka Benčina
9. Dr. Matej Holc
10. Dr. Marian Lehocky

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ORIGINAL ARTICLE

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PUBLISHED CONFERENCE CONTRIBUTION

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2. Pia Starič, Jure Mravlje, Katarina Vogel-Mikuš, Miran Mozetič, Ita Junkar, "Oxygen and nitrogen cold plasma treatment of *Fagopyrum esculentum* seeds affects seed germination rate", In: *Drugi doktorski dan Bi(o)znanosti, 27. maj 2021*, zbornik prispevkov, Biotehniška fakulteta, 2021, 95-100.

3. Ana Oberlintner, Alenka Vesel, Blaž Likozar, Uroš Novak, "Radio frequency plasma in CF4 as a fast and efficient tool for obtaining and retaining a long-term hydrophobicity of cellulose nanocrystals-reinforced chitosan films", In: *2nd International Conference on Circular Packaging, 9-10 September 2021, Slovenj Gradec, Slovenija*, Proceedings, Pulp and Paper Institute, Faculty of Polymer Technology, 2021, 287-292.

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1. Gregor Filipič, Kristina Eleršič, Darij Kreuh, Janez Kovač, Uroš Cvelbar, Miran Mozetič, *A method of colouring titanium and titanium alloys*, GB2530805 (B), Intellectual Property Office, 24. 11. 2021.
2. Ita Junkar, Rok Zaplotnik, Metka Benčina, Miran Mozetič, *Method for treatment medical devices made from nickel-titanium (NiTi) alloys*, EP3636294 (B1), European Patent Office, 17. 11. 2021.

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DEPARTMENT OF SOLID STATE PHYSICS F-5

Our research programme focuses 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 behaviour of these systems, which represent the link between perfectly ordered crystals, on the one hand, and amorphous matter, soft condensed matter and living systems, on the other. Such knowledge provides the key to our understanding of the macroscopic properties of these systems and is an important condition for the discovery and development of novel multifunctional materials, nanomaterials and biomaterials for new applications. An important part of the research programme is devoted to the development of new experimental methods and techniques in the field of magnetic resonance and magnetic resonance imaging, optical microscopy and imaging, scanning tunnelling, electronic and atomic force microscopy, as well as cold atoms and quantum technologies.

Head:
Prof. Igor Muševič

The research programme of the Department of Solid State Physics at the Jozef Stefan Institute is performed in close collaboration with the Department of Physics at the Faculty of Mathematics and Physics of the University of Ljubljana, the Institute of Mathematics, Physics and Mechanics and the Jožef Stefan International Postgraduate School. In 2021 the research was performed within three research programmes:
- Magnetic resonance and the 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 *Magnetic Resonance and Dielectric Spectroscopy of Smart New Materials* in 2021 was focused on the study of physical phenomena in condensed matter at the atomic and molecular levels. The main goal of our investigations was to discover the basic laws of physics governing the behavior of the investigated systems, from the atomic to the macroscopic levels. The attained knowledge provides a key to the understanding of the microscopic and macroscopic properties of various types of solids and is an important condition for the discovery and development of new multifunctional materials and nanomaterials for novel technological applications.

In our research we used the following complementary experimental techniques:
- Nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR) and nuclear quadrupole resonance (NQR),
- Nuclear double resonance ^{17}O–H and ^{14}N–H,
- Fast field cycling NMR relaxometry,
- Linear and non-linear dielectric spectroscopy in the range 10^{-2} Hz to 10^{9} Hz,
- Frequency-dependent ac calorimetry,
- Measurement of electrical and thermal transport coefficients,
- Magnetic measurements,
- Methods involving ultra-cold atoms.

We studied enigmatic excitations in quantum spin liquids, peculiar spin dynamics in bulk topological skyrmion lattices, investigated the electrical, magnetic and thermal properties of high-entropy alloys, used shear flow to control the shape memory of polymer-resin-dispersed liquid-crystal elastomer microparticles, and topological and caloric effects in multiferroics and soft-matter for green-energy applications and finally fullerene radical spins as qubits. Moreover, we continued to develop novel methods based on experiments with cold atoms.

The research programme was performed in close collaboration with the Department of Physics at the Faculty of Mathematics and Physics of the University of Ljubljana, the Institute of Mathematics, Physics and Mechanics, and the Jožef Stefan International Postgraduate School, as well as many recognized research groups from world-leading institutions.

In 2021 the members of the programme group published 65 original scientific papers in international peer-reviewed scientific journals and one review article. Among these, we single out an article published in *Nature Physics* (IF = 20), an article published in *Angewandte Chemie, Intl. Ed.* (IF = 15.3), an article in *Nanoscale* (IF = 7.8) and several articles in *Physical Review B* (IF = 4).

Our reasearh was directed to the following topics: quantum and topological magnetism, high-entropy alloys, functional materials, and cold atoms. Our main results are as follows:

1. Quantum and topological magnetism

Tina Arh, **Matjaž Gomilšek**, **Primož Koželj**, **Stane Vrtnik**, and **Andrej Zorko**, together with collaborators from China and Croatia, discovered magnetic ordering in the compound $Y_3Cu_9(OH)_{18}[Cl_8(OH)]$. This compound is an antiferromagnet on the distorted kagome spin lattice, which was previously believed to be magnetically disordered. However, complementary measurements of the bulk magnetization, specific heat, and magnetic torque revealed a Néel transition at 11 K. The study of high-quality crystals using optimized hydrothermal synthesis was crucial for the discovery. This suggests that the absence of the magnetic ordering in lower-quality samples is of extrinsic origin. The work was published in a paper by W. Sun et al., "Magnetic ordering of the distorted kagome antiferromagnet $Y_3Cu_9(OH)_{18}[Cl_8(OH)]$ prepared via optimal synthesis", *Phys. Rev. Mater.* **5**, 064401 (2021).

Matjaž Gomilšek, **Tina Arh**, and **Andrej Zorko**, together with a colleague from the Department of Theoretical Physics, studied the temperature dependence of dynamic spin correlations of a kagome lattice antiferromagnet. They found that even in the purely isotropic case of Heisenberg exchange interactions between nearest neighbours, chiral spin fluctuations dominate at low energies, which leads to an enhanced low-frequency response at the M point of the extended Brillouin zone. The inclusion of Dzyaloshinskii-Moriya (DM) type magnetic anisotropy leads to an anisotropic dynamic response and magnetic ordering. These theoretical predictions agree very well with measurements of inelastic neutron scattering and nuclear spin-lattice relaxation on the paradigmatic kagome antiferromagnet herbertsmithite, where the effect of DM anisotropy is small, as well as with the results of nuclear spin-lattice relaxation on the new representative of the kagome antiferromagnet $YCu_3(OH)_6Cl_3$, where, however, the effect of magnetic anisotropy is much stronger. They presented their findings in the article by P. Prelovšek *et al.*, "Dynamical spin correlations of the kagome antiferromagnet", *Phys. Rev. B* **103**, 014431 (2021).

Tina Arh and **Andrej Zorko**, together with colleagues from India and Switzerland, studied the magnetic properties of the two-dimensional spin lattice Ba_2MnTeO_6. Using complementary measurements of muon spectroscopy, magnetization and specific heat, they showed that the substance orders magnetically at a temperature of T_N = 20 K. They found that strong spin correlations are established well above the temperature of magnetic ordering, while spin dynamics remain present even in the magnetically ordered phase. Theoretical calculations have shown that this is due to the strong frustration of exchange interactions in and between the planes. They presented their findings in an article by J. Khatua *et al.*, "Development of short and long-range magnetic order in the double perovskite based frustrated triangular lattice antiferromagnet Ba_2MnTeO_6", *Sci. Rep.* **11**, 6959 (2021).

Andrej Zorko, together with colleagues from India, the USA, France, and Germany, studied the magnetic ordering of the triangular Heisenberg antiferromagnet α-HCrO$_2$ with a wide range of experimental and theoretical techniques. Despite the magnetic ordering at a Néel temperature of T_N = 22.5 K, a wide temperature range with very slow spin fluctuations was detected in the magnetically controlled phase. Since similar behaviour has previously been observed in the structurally related compounds NaCrO$_2$ and α-KCrO$_2$, such an unusual response is apparently a general characteristic of triangular antiferromagnets with ABC stacking. The results of this research were published in the article by K. Somesh *et al.*, "Universal fluctuating regime in triangular chromate antiferromagnets", *Phys. Rev. B* **104**, 104422 (2021).

Matej Pregelj, **Andrej Zorko**, and **Denis Arčon**, together with colleagues from Croatia and Switzerland, studied the dielectric response of the compound b-TeVO$_4$. They discovered a ferroelectric response of the vector-chiral magnetic ground state, where the magnitude of electrical polarization is proportional to the intensity of the magnetic reflections in neutron scattering. This suggests that the inverse Dzyaloshinskii-Moriya mechanism is responsible for the coupling between electrical polarization and magnetic order. Linear magnetoelectric coupling was not detected, but a very strong dependence of the electric coercive field on an external magnetic field was discovered, which opens the possibility of controlling recorded magnetoelectric information. They presented their findings in the article M. Dragičević *et al.*, "Control of a polar order via magnetic field in a vector-chiral magnet", *Phys. Rev. B* **104**, L121107 (2021).

Matjaž Gomilšek, in collaboration with partners from the United Kingdom and the USA, studied staggered molecular spin chains [pym–Cu(NO$_3$)$_2$(H$_2$O)$_2$] (Cu-PM; pym = C$_4$H$_4$N$_2$) and [Cu(pym)(H$_2$O)$_4$]SiF$_6$ · H$_2$O (Cu-SiF). Cu-PM is one of only a few systems with a field-induced gapped phase described by sine-Gordon (SG) quantum field theory with soliton, anti-soliton, and bound-state excitations. Using muon spectroscopy (μSR), supported by density functional theory (DFT) calculations, they discovered a transition from the SG regime to long-range order in Cu-PM at temperatures below T_N = 0.23(1) K and studied the resulting magnetic moments. No such transition was found in the chiral Cu-SiF. At temperatures above the SG spin gap both systems enter a perturbative regime with fractional spinon excitations. Using μSR the authors demonstrate that spin transport in this regime is ballistic in Cu-PM and diffusive in Cu-SiF, demonstrating the crucial impact of anisotropic perturbations on spin transport

in quantum spin chains. The work was published in the paper B. M. Huddart *et al.*, "Magnetic order and ballistic spin transport in a sine-Gordon spin chain", *Phys. Rev. B* **103**, L060405 (2021).

Matjaž Gomilšek, in collaboration with partners from the United Kingdom, studied peculiar spin dynamics in the bulk topological skyrmion lattice (SkL) systems Cu_2OSeO_3 and $Co_xZn_yMn_{20-x-y}$. Using muon spectroscopy (μSR) they found that Cu_2OSeO_3 exhibits emergent dynamic behaviour at MHz frequencies, likely due to collective SkL excitations. Complementing μSR with density functional theory (DFT) and dipolar field calculations they further demonstrated that a separate, metastable SkL phase in Cu_2OSeO_3 is unlikely to be a bulk phase and may instead be found at sample boundaries and surfaces. In $Co_8Zn_9Mn_3$ the authors observe $\sim$2 GHz excitations that reduce in frequency near the T_c of the SkL phase under various applied fields (contrasting this with thin plate results implies strong confinement effects in the latter), while in $Co_8Zn_8Mn_4$ similar behaviour is observed over a much wider range of temperatures, implying that this kind of spin dynamics persists beyond the SkL phase, raising the question of its ultimate origin. The work was published in the paper T. J. Hicken *et al.*, "Megahertz dynamics in skyrmion systems probed with muon-spin relaxation", *Phys. Rev. B* **103**, 024428 (2021).

Figure 1: Low-energy muon sites in Cu-PM identified via DFT calculations.

Matjaž Gomilšek, in collaboration with partners from the United Kingdom, studied the spin dynamics in the exotic topological spin texture materials MnNiGa and $Mn_{1.4}Pt_{0.9}Pd_{0.1}Sn$. Namely, in thin lamellae, MnNiGa was reported to host biskyrmions (topological charge N = 2 excitations, which form as bound pairs of same-chirality N = 1 Bloch skyrmions), while $Mn_{1.4}Pt_{0.9}Pd_{0.1}Sn$ was found to host antiskyrmions (N = -1 excitations with complex winding around the circumference). Using muon spectroscopy and magnetometry they revealed two spin-reorientation transitions as a function of temperature, with dynamics that slowly reduce in frequency as the upper critical temperature is approached from below. Below the lower transition, persistent spin dynamics over a broad range of frequencies are found to arise continuously in MnNiGa and more abruptly and inhomogeneously in $Mn_{1.4}Pt_{0.9}Pd_{0.1}Sn$. Unexpectedly, no conclusive dynamical evidence for biskyrmions or antiskyrmions is found in bulk samples, hinting at a possible decisive stabilizing role of confinement effects in thin lamellae samples or exotic dynamics. The work was published in the paper B. N. Wilson *et al.*, "Spin dynamics in bulk MnNiGa and $Mn_{1.4}Pt_{0.9}Pd_{0.1}Sn$ investigated by muon spin relaxation", *Phys. Rev. B* **104**, 134414 (2021).

Figure 2: (a) Phase diagram of bulk skyrmion materials. (b,c) Muon sites in Cu_2OSeO_3 identified via DFT.

Martin Klanjšek was invited by the editor of the journal Nature Physics to write a review article in the News & Views section about the progress in elucidating the ground state of the quantum magnet with the kagome lattice. This is an archetypal magnet hosting the exotic quantum spin liquid state, whose exact nature is not yet clarified. The suggested candidate states are all based on spin singlets, but it is not clear whether those are gapped or gapless. Both the recent theoretical works as well as the very recent experiments are divided between the two possibilities. The theories treating structural disorder also predict the possible coexistence of free orphan spins and spin singlets with a varying energy gap. Martin Klanjšek describes his view on the recent surprising discovery of the gradual formation of spin singlets in two quantum magnets with a kagome lattice, which is consistent with theories treating structural disorder. The article was published in M. Klanjšek, "Singlets singled out", *Nature Physics* **17**, 1081 (2021).

Figure 3: Phase diagram of bulk MnNiGa via (a) DC magnetization and (b) real part of AC susceptibility.

2. High-entropy alloys

In 2021 the research group of the Laboratory for Electrical, Magnetic and Thermal Measurements of Materials (Darja Gačnik, Andreja Jelen, Magdalena Wencka, Jože Luzar, Primož Koželj, Mitja Krnel, Stanislav Vrtnik and Janez Dolinšek) investigated the electrical, magnetic and thermal properties of high-entropy alloys (HEAs), i.e., crystalline solid solutions composed of five or more chemical elements in equi-atomic concentrations.

In the article Spin-glass magnetism of the non-equiatomic CoCrFeMnNi high-entropy alloy, **P. Koželj**, **S. Vrtnik**, **M. Krnel**, **A. Jelen**, **D. Gačnik**, **M. Wencka**, Z. Jagličić, A. Meden, G. Dražić, F. Danoix, J. Ledieu, M. Feuerbacher, **J. Dolinšek**, *J. Magn. Magn. Mater.* **523**, 167579 (2021) we investigated the magnetism of the CoCrFeMnNi HEA with random mixing of the elements on a cubic crystal lattice. We found that the material shows frustrated magnetism of a spin-glass type. We detected the memory effect, where the spin system remembers its cooling history inside the non-ergodic phase. The continuous is stopped for a macroscopic time at a certain temperature, so that the system is isothermally aged. After aging, cooling is resumed to the lowest temperature, where the temperature sweep is reversed and the zero-field-cooled (zfc) magnetization is measured upon heating in a tiny magnetic field. The zfc magnetization then shows a dip at the aging temperature and the magnitude of the dip depends on the aging time. The spin system can remember several consecutive stops at increasingly lower temperatures. The observation of the memory effect in CoCrFeMnNi HEA suggests the use of this material as a thermal memory cell for thermal storing of digital information by pure thermal manipulation, in the absence of a magnetic, electric or electromagnetic field. Figure 4 shows the
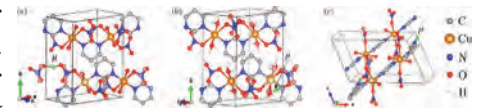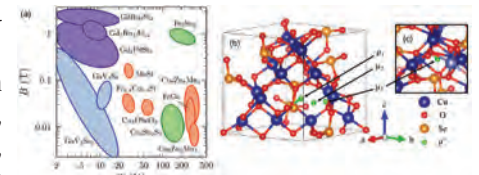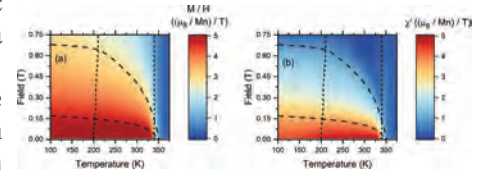

Figure 4: (a) Zfc magnetization M_{zfc} for different aging times t_w = 10 min, 30 min, 1 h, 4 h and 8 h at the aging temperature T_m = 10 K. (b) Expanded portion of M_{zfc} in the vicinity of T_m. (c) Normalized difference between the reference (unaged) curve M_zfc (t_w=0) and the aged curves, $\Delta M = [M_{zfc}(t_w=0) - M_{zfc}(t_w)]/M_{zfc}(t_w=0)$.

Figure 5: HAADF STEM micrograph and EDS elemental maps of the spinodally decomposed FeCoCrMnAl HEA.

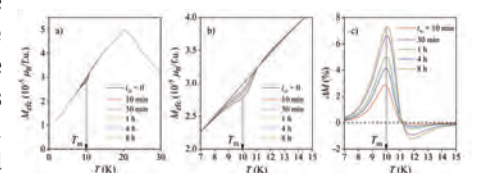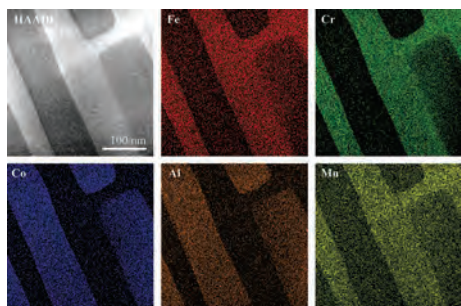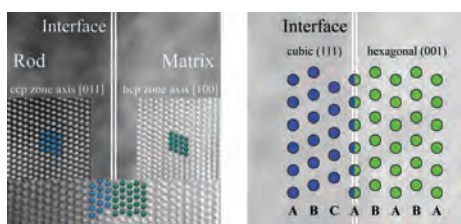*Figure 6: HAADF image of the interface region in the direct space (left panel), showing how the two phases are spatially related. The two insets in the middle show atomic-resolution projection of the ccp precipitate along the [011] zone axis and the hcp matrix along the [100] zone axis. The inset at the bottom shows the atomic structure projection of the interface. Right panel shows schematic representation of the atomic arrangement at the interface. The crystal planes of type (001) of the hexagonal matrix and (111) of the cubic precipitate are parallel to each other and one such plane represents the interface.*
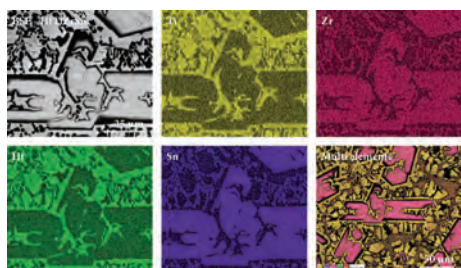

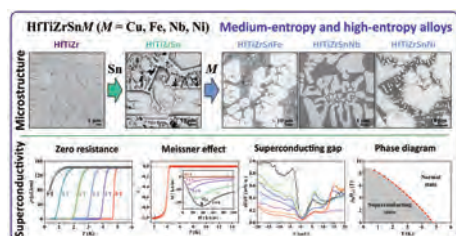*Figure 7: SEM BSE image of the HfTiZrSn HEA (upper-left panel) and EDS elemental maps.*

Figure 8: Graphs of microstructure, electrical resistivity at the superconducting transition, Meissner effect, superconducting gap in the electronic density of states at the Fermi energy and the upper critical field as a function of temperature for selected HEAs from the system HfTiZrSnM (M = Cu, Fe, Nb, Ni).

zfc magnetization during heating run, where a dip is observed at 10 K, where isothermal aging upon preceding cooling was performed for times from 10 min to 8 h.

In the paper Collective magnetism of a single-crystalline nanocomposite FeCoCrMnAl high-entropy alloy, A. Jelen, P. Koželj, D. Gačnik, S. Vrtnik, M. Krnel, G. Dražić, M. Wencka, Z. Jagličić, M. Feuerbacher, J. Dolinšek, *J. Alloys Compd*. **864**, 158115 (2021) the group investigated the collective magnetism of the FeCoCrMnAl HEA, which is spinodally decomposed into a two-phase nanocomposite structure of a bcc matrix and B2 (partially ordered bcc) nano-platelets, where each phase has a different chemical composition. Both phases contain 3*d* magnetic transition elements Fe, Co, Cr and Mn, where Fe and Co promote ferromagnetic ordering, while Cr and Mn prefer antiferromagnetic ordering. The resulting magnetism is frustrated, similar to a spin glass. EDS elemental maps of the spinodally decomposed HEA are shown in Figure 5.

In the article Nanostructure and local polymorphism in "ideal-like" rare-earths-based high-entropy alloys, A. Jelen, J.H. Jang, J. Oh, H.J. Kim, A. Meden, S. Vrtnik, M. Feuerbacher, J. Dolinšek, *Mater. Charact*. **172**, 110837 (2021) we reported the polymorphism of rare-earth-based HEAs, which were so far considered as a prototype of an "ideal" single-phase HEA with completely random mixing of the elements on a hexagonal close-packed (hcp) lattice. We have shown that despite the vanishing binary mixing enthalpies of any pair of the employed rare-earth elements (which is a condition for a completely random mixing of the elements in a solid solution), small differences in the atomic radii cause local polymorphism, where the majority matrix is hcp, whereas the elliptical precipitates with a length of several 100 nm have a cubic close-packed (ccp) structure with the same chemical composition. Figure 3 shows the hcp–ccp polymorphism in Y-Gd-Tb-Dy-Ho HEA.

In the paper Structure and Superconductivity of Tin-Containing HfTiZrSnM (M = Cu, Fe, Nb, Ni) Medium-Entropy and High-Entropy Alloys, D. Gačnik, A. Jelen, M. Krnel, S. Vrtnik, J. Luzar, P. Koželj, M. van Midden, E. Zupanič, M. Wencka, A. Meden, Q. Hu, S. Guo, J. Dolinšek, *Materials* **14**, 3953 (2021) investigated the structure, microstructure, chemical composition and superconductivity in the HEA system HfTiZrSn*M* (*M* = Cu, Fe, Nb, Ni), which contains tin, a so far unexplored element in the context of HEAs. The materials show complicated multi-phase structures. Microstructure and EDS elemental maps of the HfTiZrSn HEA are shown in Figure 7.

Superconductivity was detected in all the HEAs of the HfTiZrSn*M* (*M* = Cu, Fe, Nb, Ni) family, except the one that contains iron (Fe). Figure 8 shows the graphs of microstructure, electrical resistivity at the superconducting transition, Meissner effect, superconducting gap in the electronic density of states at the Fermi energy and the upper critical field as a function of temperature.

3. Functional materials

3.1 Shape memory in polymer dispersed liquid-crystal elastomer microparticles

Saide Umerova, Matej Bobnar, Nikita Derets, Boštjan Zalar and Andraž Rešetič in cooperation with Danjela Kuščer (K5) used shear flow to control the shape memory of polymer-resin-dispersed liquid-crystal elastomer microparticles (μLCEs). By taking advantage of the soft elastic nature of polydomain μLCEs, shear stress as a conjugate external field was successfully employed to induce the deformation and mesomorphic ordering of μLCE particles suspended in polydimethylsiloxane (PDMS), rendering them monodomain. Upon cooling from the isotropic phase down to room temperature at a high enough shear, the μLCEs have been shown to assume elongated, long-term stable geometry, exhibiting something resembling shape-memory behaviour. The elongated particles have been found to be aligned along the flow. If this alignment is lost, typically due to mixing, it can be restored using shearing in moderate flows without thermal cycling. If required, the μLCE shape memory can be erased by heating the material to the isotropic phase and then reprogrammed. This could prove to be invaluable in the additive manufacturing of elastic artefacts with a pre-programmed thermomechanical response. The work was published in a paper by S. Umerova, *et al*., Shear flow-controlled shape memory of polymer-resin-dispersed liquid-crystal elastomer microparticles, *Materials & Design* **207** 109836 (2021).

3.2 Topological and caloric effects in multiferroics and soft-matter

We continue studies of the ferroelectric properties, electromechanical and caloric effects, and energy-storage properties in novel multiferroic lead-free materials and soft matter. It was shown that these materials could be utilized in novel technologies of supercapacitors and heat-management devices. We have investigated the Halperin-Lubensky-Ma effect on nematic ordering in liquid crystals and the asymmetric lipid transfer between lipid vesicles. It was demonstrated

how nanoparticles of different shapes assemble in the defect lattices of chiral liquid-crystalline phases. B. Rožič was also professionally active in the popularization of science, **B. Rožič** *Ženske, ki spreminjajo obraz znanosti*, Slovenska nacionalna komisija za UNESCO. 2021, p. 50-51 (*Women who are changing the face of science*, Slovenian National Commission for UNESCO). Research has been disseminated in 18 scientific articles in international scientific journals, two chapters, and three invited lectures presented at international scientific meetings. Publications on multiferroics, multicalorics and soft-matter phenomena have recorded more than 600 citations in 2021 (without self-citations).

Figure 9: Schematics of shear-driven deformation and temperature 'shape resetting' of μLCEs dispersed in PDMS. The shape relaxation of the μLCEs was observed directly using polarized microscopy.

3.3. Functional nanostructures

TiO$_2$ nanostructures doped with Eu^{3+} in Nd^{3+} for temperature sensing

We continued with the investigation of TiO$_2$ nanostructures doped with lanthanide ions (Eu^{3+} and Nd^{3+}) for temperature measurements at the nanoscale. Lanthanide-based optical nanothermometers are suitable for use in biological applications as they are operating in the physiological temperature range (15 to 50 °C). TiO$_2$ was used as a support for its low toxicity and biocompatibility. TiO$_2$ nanoparticles doped with Eu^{3+} and Nd^{3+} ions were prepared using a sol-gel method. XRD, SEM, TEM, XPS and NEXFS techniques were used to determine their physiochemical characteristics. In the case of Eu^{3+} doping, the successful internalization of TiO$_2$ nanoparticles doped with Eu^{3+} ions in different cells was observed. By measuring the luminescence intensity variation of internalized doped particles, information about the cells temperature variation with a sensitivity of 0.5 K per 1% change of luminosity was obtained. Results were published in **P. Umek** et al., *Nano select* **2**, 1208 (2021) and **P. Umek** et al., *Sensors* **21** 5306 (2021).

Figure 10: Assembly of spherical nanoparticles in the disclination lines of blue phase III (left panel) and of anisotropic ones in blue phase I (right panel).

Development of a new class of polymer nanocomposites exhibiting more than ten times the enhancement of dipolar response

Dielectric polymers are pervasive in modern electrical systems due to their easy fabrication, high pliability, low dielectric loss, and high dielectric breakdown strength. However, for many electrical applications, their dielectric constant is too low. In collaboration with researchers from Pennsylvania State University we developed a new class of dielectric polymer nanocomposites, where various nanoparticles (0-D fillers) or Fe$_2$O$_3$ nanorods and Al$_2$O$_3$ nanowires (1-D fillers) are dispersed in polyetherimide (PEI). We showed that 1-D fillers at ultra-low volume loading markedly enhance the dipolar response of PEI. While nanoparticles generate a spherical shell interface nanotopology, the cylindrical shell nanostructures generated by 1-D fillers are much more efficient at raising the dipolar response in terms of extending the high dielectric response of the interfacial region and reducing the influence of low-dielectric-constant polymer regions. Consequently, PEI nanocomposites with 0.75 vol.% of nanorods exhibit more than ten times enhanced dipolar response while maintaining a low dielectric loss. These results pave the way for engineering high-performance dielectric polymers for applications over a broad temperature range.

The work was published in X. Chen, T. Yang, Q. Zhang, L. Q. Chen, **V. Bobnar**, C. Rahn, Q. M. Zhang, Topological structure enhanced nanostructure of high temperature polymer exhibiting more than ten times enhancement of dipolar response, *Nano Energy* **88**, 106226 (2021).

Development of eco-friendly cellulose-graphene oxide thin-film composites for flexible energy-storage devices

Nanocomposite films were fabricated by incorporating graphene oxide (GO) into the TEMPO-oxidized cellulose nanofibrils (TCNF), and further subjected to the UV irradiation in a nitrogen atmosphere for GO reduction. The reduction of GO and its interactions with TCNF have been proven by ATR-FTIR, FESEM, UV–Vis, Raman, and XRD spectroscopy measurements. The resulting films with an increased mechanical storage modulus are mechanically stable up to 160 °C, while due to the Maxwell-Wagner polarization the dielectric constant strongly increases even at a low GO content. Thus, these mechanically strong, flexible, and thermally stable composites are suitable, cost-effective, alternative green materials for flexible energy-storage devices. Moreover, an environmentally benign method of GO reduction by UV irradiation is a substitute for harmful chemical processes that can be extendable to other nanocomposite biomaterials.

The work was published in Y. B. Pottathara, **V. Bobnar**, Y. Grohens, S. Thomas, R. Kargl, V. Kokol, High dielectric thin films based on UV-reduced graphene oxide and TEMPO-oxidized cellulose nanofibres, *Cellulose* **28**, 3069 (2021).

Nanostructured multiferroic Pb(Zr,Ti)O$_3$–NiFe$_2$O$_4$ thin-film composites

Multiferroic thin-film composites were developed by embedding ferromagnetic NiFe$_2$O$_4$ into self-assembled porous ferroelectric Pb(Zr,Ti)O$_3$ thin films. Although bi- or multi-layers of spinel ferrites and Pb(Zr,Ti)O$_3$ were already fabricated, or, alternatively, their composites were prepared by sol-gel or RF sputtering techniques, the morphology
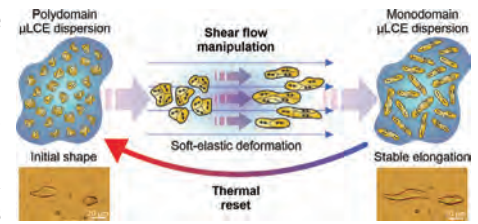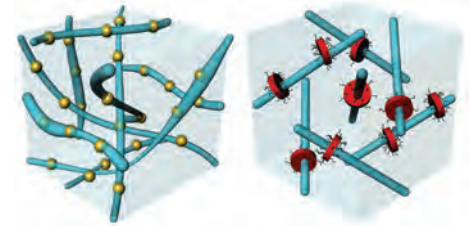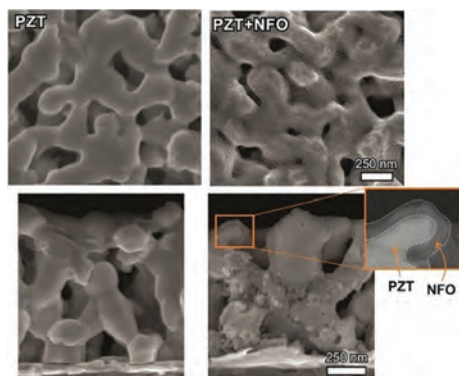
Figure 11: Structures of porous Pb(Zr,Ti)O$_3$ thin films that exhibit an extremely high piezoelectric response, and Pb(Zr,Ti)O$_3$-NiFe$_2$O$_4$ thin-film composites with an extensive contact area between the magnetostrictive and piezoelectric components. Scanning electron microscope images of film surfaces (top) and their cross-section (bottom).

of our system provides a very extensive connectivity between the magnetostrictive and piezoelectric constituents. Detailed structural investigations revealed a pure two-phase system, without any chemical reaction or solid solubility between the constituents. The multiferroicity of composites was evidenced by detecting both ferroelectric and ferromagnetic hysteresis loops. A measurable magnetic field–induced changes of the dielectric constant, not only at low frequencies but also above the characteristic frequencies of the Maxwell-Wagner behaviour, indicating a direct stress coupling between the magnetostrictive NiFe$_2$O$_4$ and piezoelectric Pb(Zr,Ti)O$_3$ grains and implies the potential utility of the developed material in magnetocapacitive applications.

The work was published in **A. Matavž**, **P. Koželj**, M. Winkler, K. Geirhos, P. Lunkenheimer, **V. Bobnar**, Nanostructured multiferroic Pb(Zr,Ti)O$_3$–NiFe$_2$O$_4$ thin-film composites, *Thin Solid Films* **732**, 138740 (2021).

3.4 Functional quantum materials

**Denis Arčon** and his colleagues from France, Germany and Greece continued their research on C$_{59}$N fullerene radicals trapped in cycloparaphenylene (CPP) rings. In the article by Y. Tanama et al., "Robust coherent spin centers from stable azafullerene radicals entrapped in cycloparaphenylene rings", *Nanoscale* **13**, 19946-19955 (2021) they investigated the mechanism of formation of stable radicals in a solid. The method of electron paramagnetic resonance showed that the formation of extremely long-lived C$_{59}$N radicals takes place in two stages and that monomeric radicals are formed only at temperatures above 150°C. The most important part of this study, however, concerned the potential use of C$_{59}$N radicals as qubits. Namely, with the method of pulsed electron paramagnetic resonance, they showed that the coherence times of such centres are extremely long and that they enable, for example, the observation of Rabi oscillations over extended time periods. The article also suggested the possible directions for the development of such materials, where complex networks of interconnected fullerene qubits could be created.

Denis Arčon and his colleagues from Tohoku University in Japan continued their research on the BaMn$_2$Pn$_2$ system (where Pn = pniktid element). These systems form the same structures as the well-known BaFe$_2$As$_2$ superconductors and are therefore also interesting from the point of view of understanding superconductivity. In two publications, T. Ogasawara et al. *Phys. Rev. B* **103**, 125108 (2021) and N. Janša et al., *Phys. Rev. B* **103**, 064422 (2021) they reported the discovery of an extremely complex temperature-dependent giant magnetoresistance. Through a combination of different experimental techniques, they have shown that a multi-orbital electronic structure is crucial for the emergence of such giant magnetoresistance. Four of the Mn 3d orbitals are important for magnetic order, while the narrow band derived from the fifth Mn 3d orbital is responsible for the transport properties themselves. It turns out that the holes in this last orbital localize below a temperature of 50 K and then form a short-range order and appear essential for the occurrence of a magnetoresisitve response.

4. Cold atoms

Katja Gosar, Tina Arh, Tadej Mežnaršič, Ivan Kvasić, Dušan Ponikvar, Tomaž Apih, Erik Zupanič, and Peter Jeglič demonstrated a novel method for detecting the gradient of a magnetic field using an elongated cloud of caesium atoms cooled to near absolute zero. Since the rotation of the atomic spins depends on the magnetic field, an image of the spin states can be used to measure how the magnetic field changes along the cloud. The gradient is determined from a single image, which is an advantage over standard methods where multiple images are needed. The method was published in K. Gosar *et al.*, "Single-shot Stern-Gerlach magnetic gradiometer with an expanding cloud of cold cesium atoms", *Phys. Rev. A* **103**, 022611 (2021).
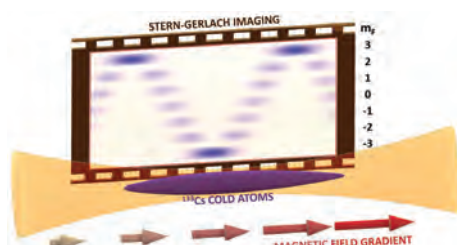

Figure 12: Illustration of the magnetic gradiometer showing a Stern-Gerlach image of an elongated caesium cold-atom cloud expanding along the laser beam.

II. Research Programme: Physics of Soft Matter, Surfaces, and Nanostructures

We demonstrated the tuneable emission of structured light from liquid-crystal (LC) microlasers and the reversible transformation of liquid-crystal droplets into fibres and objects of other shapes. We have shown that topological defects in LCs can separate the electric charge and that even spherical particles exhibit anisotropic electrostatic interactions in LCs.

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

Topological liquid-crystal superstructures as structured light lasers

Liquid crystals form an extremely rich range of self-assembled topological structures with artificially or naturally created topological defects. Liquid crystals have been used before inside laser cavities; however, until now only relatively simple liquid-crystal structures have been employed. Our study provides experimental and simulation insights into the coupling of light with the complex liquid-crystal topological superstructures inside a laser cavity. This results in non-trivial intensity and polarization of the generated structured light. The proposed soft-matter-microlaser approach opens a new direction in soft-matter photonics research. The work performed in a collaboration with the Faculty of Mathematics and Physics at the University of Ljubljana was published in the Proceedings of the National Academy of Sciences of the United States of America (PNAS 2021, DOI: 10.1073/pnas.2110839118).
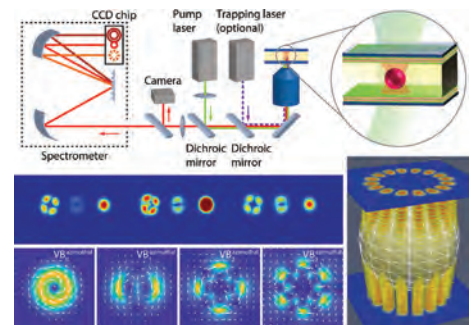

Figure 13: Optical setup used in the experiments (top) and a few examples of the experimentally generated and simulated vector laser beams (bottom).

Elasticity-driven self-shaping liquid-crystal emulsions

We present a universal concept for the shape transformation of liquid-crystal (LC) droplets suspended in aqueous surfactant solutions. The key novelty is dynamically tuning the interfacial tension to the minimum with temperature using an anionic surfactant dispersed in a LC medium and a cationic surfactant dispersed in an aqueous continuous medium. The successful reduction of the tension coupled to the tuning of the bulk LC elastic constants with the temperature drives the LC droplet into controllable self-shaping fibre structures with branches and back reversibly. We hypothesize the reversible self-shaping phenomenon is caused by the surfactant migration to the LC/water interface and forming a surfactant layer that is sensitive to temperature. The growth is induced by negative interfacial tension, which promotes a spontaneous increase of the interfacial area. Moreover, the nematic-to-SmA LC phase transition drives the fibre structures into monodispersed micro-droplets with a tuneable diameter dictated by the cooling rate. The extension of the self-shaping phenomenon in the SmC phase opens the route to generate helical fibres. Moreover, the SmA* phase shows life-like self-shaping LC shell structures analogous to the bio-membranes in living systems. A theoretical model for transforming LC emulsions into uniform fibres and vice versa is also presented. The research, performed in collaboration with researches from Gottingen, San Diego, Tokyo, and Luxembourg, was published in the PNAS, DOI: 10.1073/pnas.2011174118.
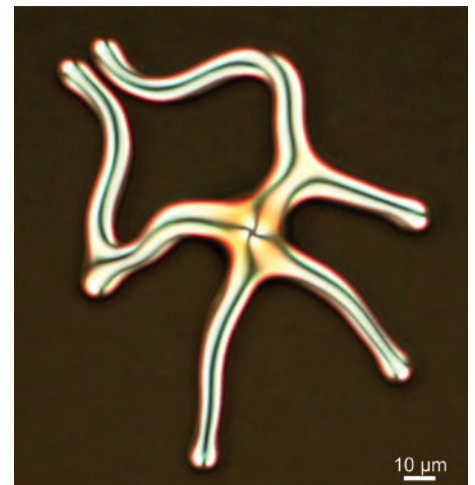

Figure 14: Self-shaping nematic fibres and droplets.

Ionically charged topological defects in nematic fluids

The ability to spatially control the electric charge is important in different fields, ranging from charged polymers, biological and active substances to colloidal materials, complex liquids and microelectronics. We showed with theoretical-simulation approaches that topological defects in nematic electrolytes can act as areas for the local separation of electric charge, forming electrically charged defective nuclei and, in selected geometries, electrical multi-layers, which is a generalization of electrical double layers in isotropic electrolytes. In particular, they showed that ions couple very efficiently with defect cores via ionic solubility, and with the surrounding orientation field through the flexoelectricity mechanism. The achievement contributes to the understanding of electrostatic mechanisms in topologically soft matter, and at the same time is a step towards understanding similar phenomena in biological systems that have a much more complex structure and composition. The research was conducted in collaboration with the Faculty of Mathematics and Physics at the University of Ljubljana and was recognized as one of the most prominent research achievements of 2021 by the Public Research Agency of the Republic of Slovenia within the program "Excellent in Science 2021" (Physical Review X 2021, DOI:10.1103/PhysRevX.11.011054).
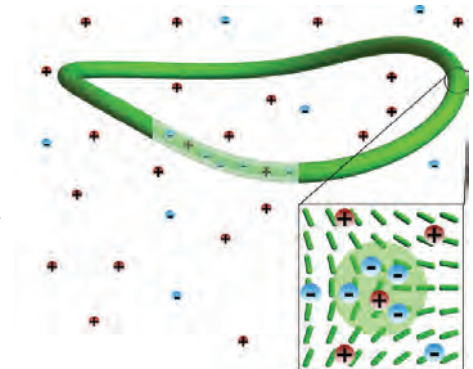
Figure 15: Ionically charged topological defects in nematic fluids.

Anisotropic electrostatic screening of charged colloids in nematic solvents

The physical behaviour of anisotropic charged colloids in nematic solvents is determined by their material dielectric anisotropy demonstrated anisotropic electrostatic screening for charged colloidal particles in a nematic electrolyte. The electrostatic potential and pair interactions decay with an anisotropic Debye screening length, contrasting the constant screening length for isotropic electrolytes. Charged dumpling-shaped near-spherical colloidal particles in a nematic medium are used as an experimental model system, demonstrating competing anisotropic elastic and electrostatic effective pair interactions for colloidal surface charges tuneable from neutral to high, yielding particle-separated metastable states. Generally, the work contributes to an understanding of electrostatic
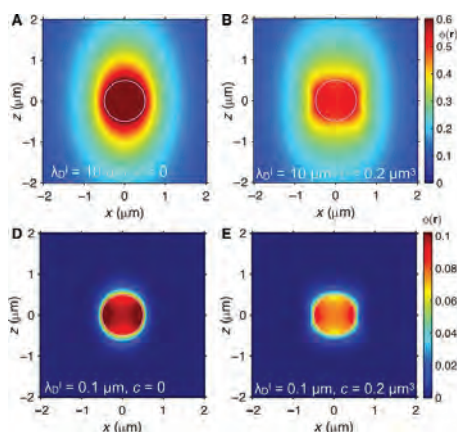
Figure 16: Anisotropic electrostatic screening of charged colloids in nematic solvents.
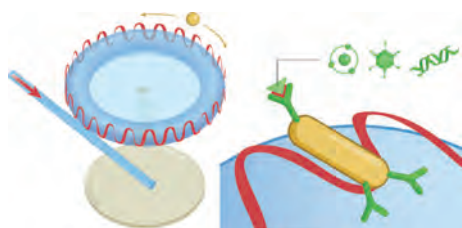

Figure 17: Principle of operation of an optical microresonator and sensing based on the binding of various molecules.
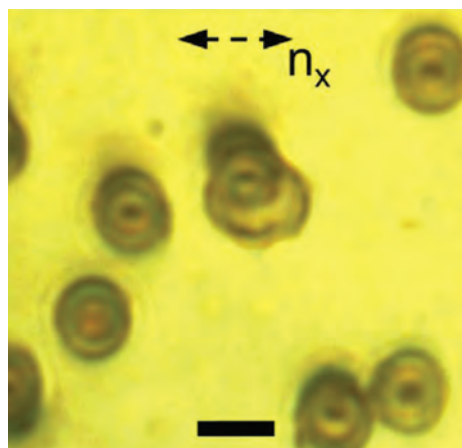

Figure 18: Microscopic texture of a DFNLC confined to microporous PET membranes.
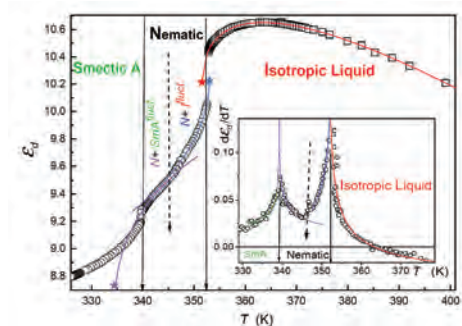

Figure 19: Dielectric response as a function of temperature.

screening in nematic anisotropic media. The research, done in collaboration with researchers from Physics at Universities of Ljubljana and Boulder, was published in Science Advances 2021, DOI: 10.1126/sciadv.abd0662.

Whispering-gallery-mode sensors for biological and physical sensing

In a review paper published in Nature Reviews Methods Primers we, in the collaboration with researchers from the Universities of Exeter, Michigan, and Okinawa, introduce whispering-gallery-mode microcavities in different geometries, such as microspheres, microtoroids, microcapillaries and microrings. Whispering-gallery-mode microcavities are miniature micro-interferometers that use the multiple-cavity passes of light for very sensitive measurements at the microscale and nanoscale, including single-molecule and ion measurements. We describe sensing mechanisms, including mode splitting and resonance shift, and optomechanical and optoplasmonic signal transductions. Applications and experimental results cover in-vivo and single-molecule sensing, gyroscopes and microcavity quantum electrodynamics (*Nat Rev Methods Primers* 2021, DOI: 10.1038/s43586-021-00079-2).

Dual-frequency electrically driven nematic microstructures confined to biaxial porous polymer membranes

We report a study of internal ordering and the electro-optical response of dual-frequency nematic liquid crystals (DFNLCs) confined to microporous polyethylene terephthalate (PET) membranes. The DFNLCs are characterized by positive/negative signs of dielectric anisotropy in low/high-frequency electric fields. Low/high-frequency electric fields were applied to the PET-DFNLC membrane to manipulate the internal nematic configuration. We found that the low/high-frequency electric fields drive a structural transformation resulting in the suppressed/increased propagation of near-infrared electromagnetic radiation through a composite material. The results are discussed for photonic applications. The study has been performed in collaboration with researchers from Moscow and published in Applied Physics Letters 2021, DOI: 10.1063/5.0069056.)

Pretransitional Effects of the Isotropic Liquid–Plastic Crystal Transition

We report on strong pretransitional effects across the isotropic liquid–plastic crystal melting temperature in linear and nonlinear dielectric response. Studies were carried out for cyclooctanol in the unprecedented range of temperatures 120 K < T < 345 K. Such pretransitional effects have not yet been reported in any plastic crystals. We compare the observed pretransitional behaviour with the one observed in 8OCB (a typical liquid-crystal representative), displaying a reversed sequence of phase transitions in orientational and translational degrees of order on varying the temperature. Furthermore, in its nematic phase, we demonstrate the first-ever-observed temperature-driven crossover between regions dominated by an isotropic liquid and smectic A pretransitional fluctuations. We propose a pioneering minimal model describing plastic crystal phase behaviour where we mimic the derivation of classical Landau-de Gennes-Ginzburg modelling of Isotropic-Nematic-Smectic A LC phase behaviour. The study has been performed in collaboration with researchers from Warsaw and published in Molecules 2021*, DOI:* 10.3390/molecules26020429.

Co-revolving topological defects in a nematic liquid crystal

A patterned surface defect of strength m = 1 and its associated disclination lines can decompose into a pair of surface defects and disclination lines of strength m = 1/2. For a negative dielectric anisotropy liquid crystal subjected to an applied ac electric field *E*, these half-integer defects are observed to wobble azimuthally for *E* less than some threshold field and, for sufficiently large fields, to co-revolve antipodally around a central point approximately midway between the two defects. This behaviour is elucidated experimentally as a function of the applied field strength and frequency. A complete field vs. frequency "phase diagram" compellingly suggests that the induced fluctuations and eventual co-revolutions of the defects are driven by the hydrodynamic instability. The observed behaviour suggests a Lehmann-like mechanism that drives the co-revolution. The study was made in collaboration with researchers from Cleveland (Soft Matter 2021*, DOI:* 10.1039/D1SM01124C).

Minimum dissipation theorem for microswimmers

Biological or artificial microswimmers propel themselves through a fluid in the low-Reynolds-number regime either by periodically changing their shape or by inducing an effective slip velocity along their surface. We have

derived a minimum dissipation theorem for microswimmers. It provides a lower bound on the power needed by an active swimmer, expressed with the drag coefficients of two passive bodies of the same shape: one with a no-slip and one with a perfect-slip boundary. The theorem holds for swimmers of any shape, moving with any translational and/or rotational velocity. The proof involves a generalization of the Helmholtz minimum dissipation theorem, the principle of linear superposition and the Lorentz reciprocal theorem. We also show that the optimal swimmer has the velocity profile of the perfect-slip body (e.g., a gas bubble) and the tangential traction of the no-slip body. We have thus reduced a seemingly complex optimization problem to the calculation of two passive drag coefficients. The study was mostly performed at the Max Planck Institute for Dynamics and Self-Organization in Göttingen (Phys. Rev. Lett. 2021, DOI: 10.1103/PhysRevLett.126.034503).

Figure 20: Surface topology nucleated disclinations.

Ciliary chemosensitivity is enhanced by cilium geometry and motility,

Primary cilia, which are usually immotile, have primarily sensory functions as receptors for chemical or mechanical signals. However, there is mounting evidence that the sensory functions are not limited to immotile cilia and that beating cilia can also contain chemical receptors. This raises the question as to whether there is a physical advantage in placing chemical receptors on a cilium in terms of sensitivity. To answer this question, we studied the capture rates of signalling particles on a model cilium embedded in a flat surface. We showed that, even in a quiescent fluid with no advection, the cilium already achieves the same capture rate as a surface patch with 4 times the surface area. When the cilium is placed in an external shear flow, the equivalent surface ratio rises to 6 times. A motile cilium can achieve a significant enhancement of the capture rate at high Péclet numbers, but only if it beats in a non-reciprocal way and thus induces a long-range net flow in the surrounding fluid. When many immotile cilia are placed in proximity, the capture rate per cilium is reduced because of the depletion of the concentration field. However, when the same cilia beat asymmetrically, their capture rate is enhanced by the flow generated by the surrounding cilia. The study was mostly performed at the Max Planck Institute for Dynamics and Self-Organization in Göttingen (eLife 2021, DOI: 10.7554/eLife.66322).

Figure 21: The optimal active microswimmer can be represented as a superposition of the flow around a perfect slip body and that around a no-slip body (shown for a spherical swimmer).

New W_nO_{3n-1} stoichiometric phase

We synthesized and characterized tungsten suboxide crystals, which grow in the form of nanotiles. Three new stoichiometric phases were determined from high-resolution TEM images: $W_{13}O_{38}$ ($WO_{2.923}$), $W_{12}O_{35}$ ($WO_{2.917}$) in $W_{11}O_{32}$ ($WO_{2.909}$). The experimental unit-cell parameters were in agreement with the calculated ones. The nanotiles have a distinct zig-zag morphology, with corrugation that are several 10 nm deep. The valence band spectrum showed some density of states at the Fermi energy, making the material slightly metallic (Nanomaterials 2021, DOI: 10.3390/nano11081985).

Figure 22: The particle capture rate per cilium (length of red bars) for: (a) an isolated immotile cilium, (b) a group of 7 immotile cilia, (c) an isolated beating cilium and (d) a group of 7 beating cilia. While the capture rate in a group of immotile cilia is reduced due to depletion, motile cilia benefit from mutual enhancement by the generated flow.

Filtration efficiency of respiratory masks used during the COVID-19 pandemic

We performed size- and time-dependent filtration-efficiency measurements of face masks and improvised respiratory protection equipment used during the COVID-19 pandemic. The results showed the high filtration efficiency of FFP2, FFP3, and certified surgical masks for all sizes of tested particles, while the filtration efficiency of washable masks depended on their constituent fabrics. The filtration efficiency for the FFP2 fabric was above 98.6%, while for the FFP3 fabric it was above 99.9%. Similar or slightly lower filtration-efficiency values were observed for tested materials obtained from different surgical masks. Different cotton materials that are usually used in cotton masks had the filtration efficiency between 26% and 82%, mainly due to the large diameter of the cotton fibres, which also lack any static charge. The study was done in collaboration with researchers from the Department of Physics at the University of Ljubljana and industry (Sensors 2021, DOI: 10.3390/s21051567).

Figure 23: The WO_{3-x} plates in a form of nanotiles.

Tuning graphene doping by carbon monoxide intercalation at the Ni(111) interface

Under near-ambient pressure conditions, carbon monoxide molecules intercalate underneath an epitaxial graphene monolayer grown on Ni(111), getting trapped into the confined region at the interface. On the basis of ab-initio density functional theory calculations, we provided a full investigation of the intercalated CO pattern, highlighting the modifications induced on the graphene electronic structure. The most relevant signature of the CO intercalation is a clear switching of the graphene doping state, which changes from n-type, when strongly interacting
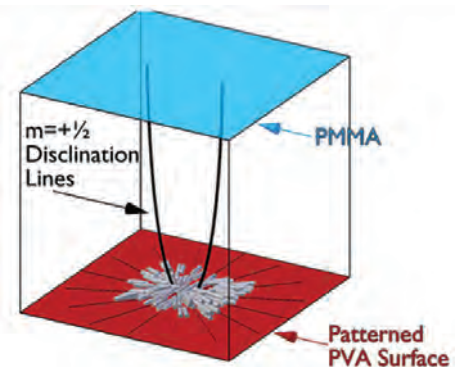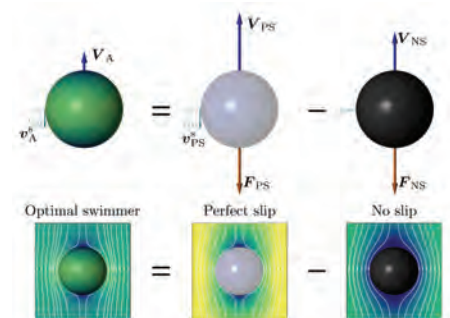

Figure 24: Schematic representation of the measurement of filtration efficiency for respiratory masks during the COVID-19 pandemic.

Figure 25: Carbon monoxide intercalated at a graphene/Ni(111) interface forms periodic patterns, decouples the graphene from the Ni(111) and shifts the Dirac cone up to about 1 eV.
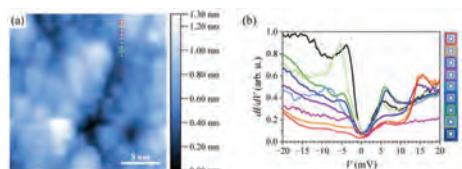
Figure 26: Topographic STM image of the HTZS-Nb sample surface and the corresponding dI/dV curves showing a varying superconducting gap.
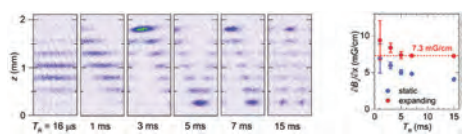
Figure 27: (a) Absorption images of position-dependent mF-state populations for a range of interrogation times and (e) the extracted component of the magnetic-field gradient.
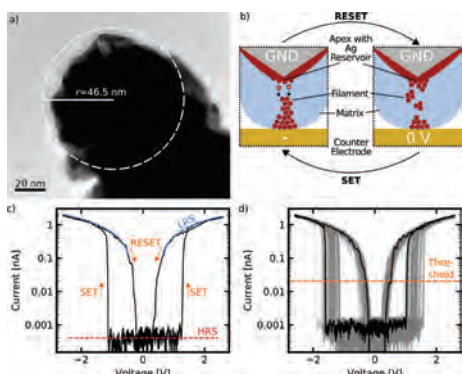
Figure 28: (a) TEM image of a memtip indicating a radius of curvature of 46.5 nm. (b) Schematics of SET and RESET operations. The current in the low resistive state (LRS) is limited by the 1-GΩ serial resistor incorporated into the experimental setup. The high resistance state (HRS) is given by the detection limit of the setup. (c) and (d) Representation of a single and 100 sequential cycles showing a consistent switching window. A threshold level of 20 pA, as indicated, is chosen for a reliable detection of SET and RESET.

with the metal surface, to p-type. The shift of the Dirac cone linearly depends on the CO coverage, reaching about 0.9 eV for the saturation value of 0.57 ML. Theoretical predictions are compared with the results of STM, LEED and XPS experiments, which confirm the proposed scenario for the nearly saturated intercalated CO system. The paper was published in collaboration with groups from Italy (*Carbon 2021*, DOI: 10.1016/j.carbon.2021.01.120).

Structure and Superconductivity of Tin-Containing HfTiZrSnM (M = Cu, Fe, Nb, Ni) Medium-Entropy and High-Entropy Alloys

In an attempt to incorporate tin into high-entropy alloys composed of the refractory metals Hf, Nb, Ti and Zr with the addition of the 3d transition metals Cu, Fe, and Ni, we synthesized a series of alloys in the system HfTiZrSnM (M = Cu, Fe, Nb, Ni). The alloys were characterized crystallographically, microstructurally, and compositionally, and their physical properties were determined, with the emphasis on superconductivity. A common feature of the alloys is a microstructure of large crystalline grains of a hexagonal (Hf, Ti, Zr)5Sn3 partially ordered phase embedded in a matrix that also contains many small inclusions. Based on the electrical resistivity, specific heat, and magnetization measurements, a superconducting (SC) state was observed in the HfTiZr, HfTiZrSn, HfTiZrSnNi, and HfTiZrSnNb alloys. The HfTiZrSnFe alloy shows a partial SC transition, whereas the HfTiZrSnCu alloy is non-superconducting. A paper was published in collaboration with groups from Poland, China and Sweden (*Materials, 2021*, DOI: 10.3390/ma14143953).
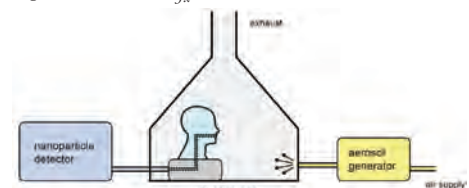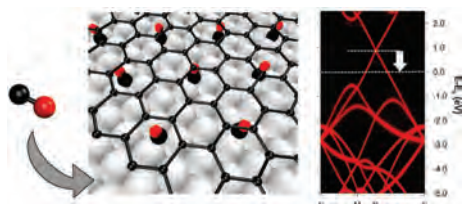
Single-shot Stern-Gerlach magnetic gradiometer with an expanding cloud of cold caesium atoms

We combined the Ramsey interferometry protocol, the Stern-Gerlach detection scheme, and the use of the elongated geometry of a cloud of fully polarized cold caesium atoms to measure the selected component of the magnetic-field gradient along the atomic cloud in a single shot. In contrast to the standard method where the precession of two spatially separated atomic clouds is simultaneously measured to extract their phase difference, which is proportional to the magnetic-field gradient, we show a gradiometer using a single image of an expanding atomic cloud with the phase difference imprinted along the cloud. Using resonant radio-frequency pulses and Stern-Gerlach imaging, we first demonstrate nutation and Larmor precession of atomic magnetization in an applied magnetic field. Next, we let the cold atom cloud expand in one dimension and apply the protocol for measuring the magnetic-field gradient. The resolution of our single-shot gradiometer is not limited by the thermal motion of atoms and has an estimated absolute accuracy of better than ±0.2 mG/cm (±20 nT/cm). (*Phys. Rev. A, 2021*, 10.1103/PhysRevA.103.022611)

Correlations and filamentary dynamics in nanoscale memristor

To emulate the neural dynamics of excitatory and inhibitory processes, memristors offer a practical hardware approach to implement such functionalities for possible utilization in efficient probabilistic computation. In an attempt to unravel the intrinsic long-range dynamics at room temperature, while mitigating the unwanted thermal drift, we focus on nanoscale memristor built at the apex of a scanning probe tip. With the design of such functionalized cantilevers (entitled here as "memtips") we captured the long-term intrinsic current response, identified temporal correlations between switching events and observed emerging spiking dynamics directly at the nanoscale. Utilization of an identical memtip for measurements on different counter electrodes made it possible to directly compare the impact of different device configurations on the switching behaviour of the same filament. Such an analytical approach in ambient conditions will pave the way towards a deeper understanding of filamentary switching phenomena on the nanoscale. The study was conducted in collaboration with researchers from the University of Kiel and published in *Nanomaterials* **2021**, DOI: 10.3390/nano11020265.

III. Research programme: Experimental biophysics of complex systems and imaging in biomedicine

The programme group **Experimental biophysics of complex systems and imaging in biomedicine** combines research of the processes and structures of biological systems by developing new, advanced experimental techniques of super-resolution microscopies, microspectroscopies and nanoscopies as well as new imaging techniques. Our research is mainly focused on the response of molecular and supramolecular structures to interactions between materials and living cells as well as between light and living cells. We are interested in molecular events and physical

mechanisms with which these events are causally connected, time scales, conditions and applied value of the investigated mechanisms, especially for use in medicine and in the field of healthcare in general. With the development of new, coupled, super-resolution and spectroscopic techniques we want to open new possibilities to investigate

biological systems and from there onwards to open new possibilities for designing medical materials and devices, for diagnostics, therapy and tissue regeneration, representing key challenges due to the population aging. The investment into the new super-resolution STED system opened a variety of fluorescence microscopy approaches: STED microscopy and two-photon (2PE) microscopy, multichannel spectrally resolved fluorescence lifetime imaging (spFLIM), fluorescence microspectroscopy (FMS). These, coupled with optical tweezers, can be used to examine the interactions between

After founding the spin-off company Infinite d.o.o. on the basis of our own breakthrough ideas, the company acquired its first start-up investment in 2021, and with it already supported further basic and applied research in the field of disease-triggering mechanisms.

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

In 2018, in Nano Letters, we proposed a causal link between the inhalation of nanoparticles and cardiovascular disease based on the presence of coagulation enzymes tissue factor, factor X, and plasma membrane lipids in the corona of TiO_2 nanoparticles after exposure to lung epithelial cells. To further **elucidate the role of lipids in the activation of factor X**, we used soluble forms of PS and PE (1,2-dicaproyl-sn-glycero-3-phospho-l-serine (C6PS), and 1,2-dicaproyl-sn-glycero-3-phospho-ethanolamine (C6PE). We found that two molecules of each lipid bind independently to factor VIIa, with a dissociation constant of around 150 μM, increasing the rate of activation of factor X by about 100-fold in the presence of a soluble tissue factor. The work was published in Podlipec, Rok, Mur, Jaka, Petelin, Jaka, Štrancar, Janez, Petkovšek, Rok. Method for controlled tissue theranostics using a single tunable laser source. Biomedical optics express, ISSN 2156-7085, 2021, vol. 12, no. 9, pp. 5881-5893, doi: 10.1364/BOE.428467.

To prevent experimental artefacts by poorly fluorescently labelled metal oxide nanoparticles – the largest subpopulation of nanoparticles by industrial production and applications – in live-cell imaging, we introduced a **set of experimental methods to enable artefact-free fluorescent labelling** and demonstrated its application in the case of TiO_2 nanotubes. We characterized potential changes of the nanoparticles' surface charge and morphology that might occur during labelling by using zeta-potential measurements and transmission electron microscopy and assessed the stable binding of the fluorescent dye to the nanoparticles with either fluorescence intensity measurements or fluorescence correlation spectroscopy, which ensures reliable nanoparticle localization within living cells. The work was published in Kokot, Boštjan, Kokot, Hana, Umek, Polona, Van Midden, Katarina Petra, Pajk, Stane, Garvas, Maja, Eggeling, Christian, Koklič, Tilen, Urbančič, Iztok, Štrancar, Janez. How to control fluorescent labeling of metal oxide nanoparticles for artefact-free live cell microscopy. Nanotoxicology, ISSN 1743-5404, 2021, vol. 15, no. 8, pp. 1102-1123, doi: 10.1080/17435390.2021.1973607.

Within the industrial cooperation with our spin-out company Infinite d.o.o. we have enabled the live observation of **new**, **early molecular events** followed by exposure of our in-vitro lung barrier. We have identified some events that appear **earlier than the quarantine of nanomaterials** and could become the key events for the even faster prediction of long-term health complications. Among them, we discovered the surfing nanomaterials and gap formation, for which we are still looking for the causal connections with other known events. In addition, we have **upgraded the back-scattered microscope detection of particulate matter** on the fluorescence microscopes to enable label-free tracking of particles.

As a part of two PhD research projects, we have firstly developed **the novel concept of dose**, which advances the concept of local dose including the information on local interactions. Secondly, we have observed nanomaterial-triggered changes in neurons', where the importance of **immune cells** was even greater than in the case of lung barrier exposure. The latter seem to be **crucial for the survival of neurons**. These two doctoral dissertations will be defended in 2022.

Successful research work conducted within the framework of the ARRS project Spatial and temporal design of laser light for minimally invasive ophthalmic procedures (L2-9254), was rewarded with the publication in the first-quartile journal Biomedical Optics Express [1]. The study reports on **a new teranostic method for detecting the effect of laser therapy on ocular tissues** in real-time based on measurements and the **analysis of fluorescence lifetime** and the use of a **powerful adaptive 2-photon laser system** developed in the Laboratory of Photonics and Laser Systems (FOLAS), Faculty of Mechanical Engineering, University of Ljubljana. For the research work within the ARRS project L7-7561, an official publication was rewarded to the granted European patent (EP3755994B1)

Štrancar, Janez, Podlipec, Rok, Urbančič, Iztok, Arsov, Zoran, Vrečko, Andrej. Image-processing apparatus and image-processing method for detection of irregularities in tissue: European patent specification EP 3 755 994 B1, 2021-05-26. Munich: European Patent Office, 2021. 23 pp.,

In cooperation with the Laboratory of Thermal Engineering (LTT), Faculty of Mechanical Engineering and the Department of Pharmaceutical Chemistry, Faculty of Pharmacy, we conducted new studies for the detection and analysis of temperature dynamics in the micro-boiling processes with new preparation methods and new combinations of the developed temperature-sensitive organic and inorganic molecules. Based on the results of the research, we are preparing a scientific publication planned for 2022.

Within the Crossing Borders and Scales (CROSSING) project, we continued to study new approaches and **optimize protocols for correlative microscopy** on relevant biological systems using new high-resolution microscopes and spectroscopes (synchrotron soft XRF, cryo micro-PIXE, etc.) with the ongoing ones. To study the mechanisms that lead to chronic inflammation of the lung epithelium due to nanoparticle exposure, we added time-dynamics measurements with high-resolution HIM microscopy in addition to the temporal dynamics of the interaction measured on living systems. The results of the study will be published in 2022 in a journal with a high impact factor. In collaboration with the Department of Low and Medium Energy Physics (F2) and the Department of Orthopedics, University Medical Center Maribor, we conducted a study to understand the negative impact of the metal wear debris from hip prosthesis on the surrounding tissue, potentially leading to an immune response. Using some of the most advanced high-resolution and sensitive microscopes and spectroscopes available at the JSI and HZDR, we directly identified, among other things, wear-debris-induced oxidative stress, which can cause chronic inflammation. All the findings were published in Podlipec, Rok, Punzón Quijorna, Esther, Pirker, Luka, Kelemen, Mitja, Vavpetič, Primož, Kavalar, Rajko, Hlawacek, Gregor, Štrancar, Janez, Pelicon, Primož, Fokter, Samo K. Revealing inëammatory indications induced by titanium alloy wear debris in periprosthetic tissue by label-free correlative high-resolution ion, electron and optical microspectroscopy. Materials, ISSN 1996-1944, 2021, vol. 14, issue 11, pp. [1-16], doi: 10.3390/ma14113048.]. Using complementary imaging methods, we also participated in a published study focused on the effects of toxic nanoparticles on freshwater organisms in Schymura, Stefan, Drev, Sandra, Podlipec, Rok, Rijavec, Tomaž, Lapanje, Aleš, Štrok, Marko, et al. Dissolutionbased uptake of nanoparticles by freshwater shrimp: a dual-radiolabelling study of the fate of anthropogenic cerium in water organisms. Environmental science, Nano, ISSN 2051-8161, 11 pp., doi: 10.1039/d1en00264c.

We kept developing advanced microscopy and microspectroscopy techniques and applied them to elucidate diverse molecular and cellular mechanisms. We used Eu-doped TiO_2 nanoparticles as intracellular temperature sensors, as described in Urbančič, Iztok et al. Aggregation and mobility of membrane proteins interplay with local lipid order in the plasma membrane of T cells. FEBS Letters. [Online ed.]. [in press]2021, 20 pp. ISSN1873-3468. DOI: 10.1002/1873-3468.14153. In collaboration with the University of Oxford (UK), we unravelled how **membrane lipids and proteins interplay to support the activation of T cells**; the contribution was featured as the cover story of the renowned journal *FEBS Letters* Havrdová, Markéta, Urbančič, Iztok, Bartoň Tománková, Kateřina, Malina, Lukáš, Štrancar, Janez, Bourlinos, Athanasios B. Self-targeting of carbon dots into the cell nucleus: diverse mechanisms of toxicity in NIH/3T3 and L929 cells. International journal of molecular sciences. 2021, vol. 22, no. 11, pp. 5608-1-5608-16. ISSN 1661-6596. DOI: 10.3390/ijms22115608. With partners from the University of Olomouc (CZ), we investigated the **uptake of carbon nanodots as potential cancer therapeutics** Biagiotti, Giacomo, Purić, Edvin, Urbančič, Iztok, Krišelj, Ana, Weiss, Matjaž, Mravljak, Janez, Gellini, Cristina, Lay, Luigi, Chiodo, Fabrizio, Anderluh, Marko, et al. Combining cross-coupling reaction and Knoevenagel condensation in the synthesis of glyco-BODIPY probes for DC-SIGN super-resolution bioimaging. Bioorganic chemistry. 2021, vol. 109, pp. 1-10, ilustr. ISSN 0045-2068, DOI: 10.1016/j.bioorg.2021.104730. We participated in the development of a new fluorescent probe to stain immune cells that is capable of super-resolution STED microscopy, published in Kokot, Boštjan, Kokot, Hana, Umek, Polona, Van Midden, Katarina Petra, Pajk, Stane, Garvas, Maja, Eggeling, Christian, Koklič, Tilen, Urbančič, Iztok, Štrancar, Janez. How to control the fluorescent labelling of metal oxide nanoparticles for artefact-free live cell microscopy. Nanotoxicology, ISSN 1743-5404, 2021, vol. 15, no. 8, pp. 1102-1123, doi: 10.1080/17435390.2021.1973607.
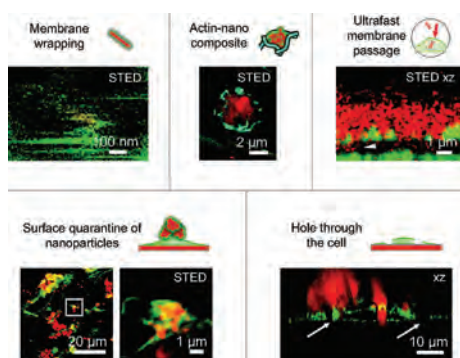
Figure 29: Examples of five early molecular events in living epithelial cells following exposure to nanomaterial (TiO_2 nanotubes labelled, red), detected with confocal or STED fluorescence microscopy. Other channels are context-related (green).

Study of magnetoliposomes as MRI contrast agents and drug-delivery systems

The Laboratory of Magnetic Resonance Imaging with our partners from the Department of Nanostructured Materials (K7, JSI) and international partners conducted a larger study on the effect of PD1 blockade on the therapeutic efficacy of novel doxorubicin-loaded temperature-sensitive liposomes. Studied were low temperature-sensitive magnetoliposomes for efficient drug delivery that can be photothermally activated. These magnetoliposomes also act as contrast agents for magnetic resonance imaging. The magnetoliposomes were prepared by embedding coated

iron oxide nanoparticles (IO NPs) in the lipid bilayer of liposomes and loading the liposimes with the drug Doxorubicin. Our role in the study was to characterize the NMR relaxation properties of the magnetoliposomes and to image their accumulation in tumours of mice. It turned out that these magnetoliposomes are efficient T_2 NMR relaxation contrast agents with high transverse r_2 relaxivity of 333 mM^{-1} s^{-1}. Excellent contrast agent properties of the magnetoliposomes enables efficient MRI guidance of the drug delivery and therefore better and more efficient tumour therapy. The results of this study were published in a well-renowned journal in an article Ma Guanglong, Kostevšek Nina, Markelc Boštjan, Hudoklin Samo, Erdani-Kreft Mateja, Serša Igor, Čemažar Maja, Marković Katarina, Ščančar Janez et al. PD1 blockade potentiates the therapeutic efficacy of photothermally-activated and MRI-guided low temperature-sensitive magnetoliposomes. *Journal of controlled release*, ISSN 0168-3659, 2021, vol. 332, 45 pp., pp. 419-433, doi: 10.1016/j.jconrel.2021.03.002. We were also included in a similar study where instead liposomes erythrocyte membranes with embedded iron oxide nanoparticles were used. This study was published in an article: Kostevšek Nina, Miklavc Patricija, Kisovec Matic, Podobnik Marjetka, Al-Jamal Wafa, Serša Igor. Magneto-erythrocyte membrane vesicles' superior T_2 MRI contrast agents to magnetoliposomes. *Magnetochemistry*, ISSN 2312-7481, 2021, vol. 7, no. 4, pp. 51-1-51-14, doi: 10.3390/magnetochemistry7040051.

Magnetic resonance imaging of wood. Changes of the water state and its distribution in a beech sample while drying from the green (fresh cut) to the absolutely dry state were monitored by one-dimensional and two-dimensional ^{1}H NMR relaxometry as well as by spatial mapping of the NMR relaxation times T_1 and T_2. We found that the relaxometry results were consistent with the model of homogeneously emptying pores in a bioporous system with connected pores. This was also confirmed by the relaxation-time mapping results, which revealed the moisture transport in the course of drying from an axially oriented early- and latewood system to radial rays through which it evaporates from the branch. The results of this study confirmed that MRI is an efficient tool to study the pathways of water transport in wood while drying and is capable of determining the state of water and its distribution in wood. This study was published in an article: Mikac Urška, Merela Maks, Oven Primož, Sepe Ana, Serša Igor. MR study of water distribution in a beech (Fagus sylvatica) branch using relaxometry methods. *Molecules*, ISSN 1420-3049, 2021, vol. 26, no. 14, pp. 4305-1-4305-10, doi: 10.3390/molecules26144305. In addition to this study, we participated in another study on wood where we investigated the efficiency of the suppression of non-native tree species by stem wounding using incomplete girdling. This type of injury causes the plant to lose its vitality, become weaker after the first year and then die within a few years. Our task was to image the moisture distribution in the mechanically wounded stem. This study was published in an article: Plavčak Denis, Mikac Urška, Merela Maks. Influence of mechanical wounding and compartmentalization mechanism on the suppression of invasive plant species using the example of Cherry Laurel (Prunus laurocerasus). *Forests*, ISSN 1999-4907, 2021, vol. 12, iss. 2, 1-15 pp., ISSN 1999-4907, DOI: doi.org/10.3390/f12121646.

Correlations between the treatment outcome of ischemic stroke patients with X-ray properties of their thrombi. All the patients with a suspected stroke are directed to a whole-brain CT scan, which is used to look for early features of ischemia to locate the occlusion and its size, while the Hounsfield Units (HUs) values of the thrombus causing the stroke are usually overlooked. In this study we demonstrated that the HUs value is relevant and can help in better treatment planning for a stroke. The study included patients diagnosed with ischemic stroke in the middle cerebral artery (MCA). In all patients, systemic thrombolysis was not successful, and mechanical recanalization was needed. The retrieved thrombi were also analysed histologically for the determination of the red blood cells (RBCs) proportion. The CT scan of the proximal MCA segment was analysed for the average HU value and its variability both in the occluded section and the symmetrical normal site. Relevant positive correlations were found between the average HU value of thrombus and the treatment outcome evaluated by modified Rankin Scale (mRS), initial mRS, number of passes with thrombectomy device as well as RBC proportion. This study was published in an article: Viltužnik Rebeka, Vidmar Jernej, Fabjan Andrej, Jeromel Miran, Miloševič Zoran, Kocijančič Igor, Serša Igor. Study of correlations between CT properties of retrieved cerebral thrombi with treatment outcome of stroke patients. *Radiology and oncology*, ISSN 1318-2099. 2021, vol. 55, iss. 4, 409-417 pp., doi: 10.2478/raon-2021-0037.
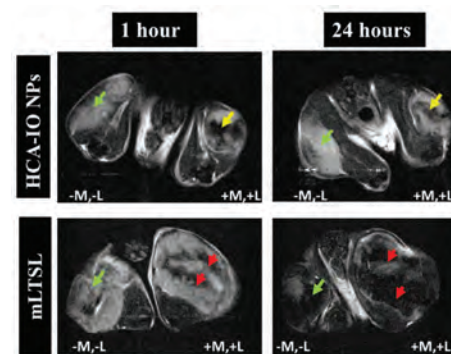
Figure 30: Low-temperature-sensitive magnetoliposomes as efficient T_2 NMR contrast agents in vivo. CT26 tumour-bearing mice were intravenously injected with coated iron oxide nanoparticles (HCA-IO NPs) or with low-temperature-sensitive magnetoliposomes with embedded coated iron oxide nanoparticles (mLTSL) at a Fe dose of 50 μg per mouse. After injection, one tumour was immediately taped with a magnet for 50 min and irradiated with the laser (808 nm, 0.3 W/cm2) for 10 min (+M, +L). The second tumour was not exposed to a magnet and was not irradiated (-M, -L). T_2-weighted images were taken 1 h and 24 h post-injection. Red and yellow arrows indicate darker contrast in treated tumours (+M, +L) injected with mLTSL and HCA-IO NPs, respectively. Green arrows indicate non-treated tumours (-M, -L). T_2-weighted MR images were recorded using the spin-echo sequences with parameters TE/TR = 40/3000 ms.
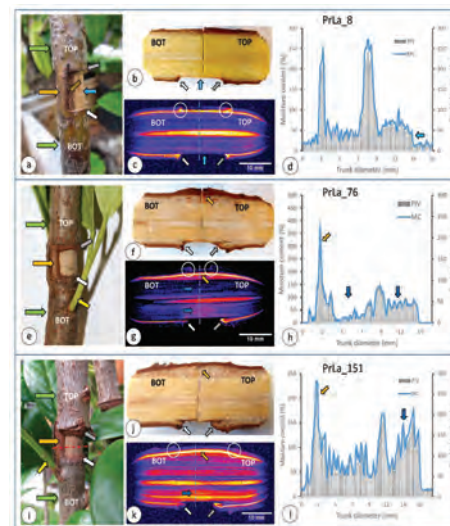
Figure 31: Injured stems of cherry laurel (Prunus laurocerasus) at day 8, 76 and 151 after mechanical wounding: (a,e,i) situation on the day of sampling; (b,f,j) bisected samples on the bottom (BOT) and top (TOP) part; (d,h,l) radial profile of moisture content calculated from MRI pixel intensity values, (c,g,k) Magnetic Resonance Image (MRI) of injured stems.

MRI as a tool for monitoring the response of tissues to a pulsed electric field treatment. The aim of this study was to investigate the permeabilization of cell membranes in plant and animal foods (potatoes, apples, chicken) resulting from a treatment with a pulsed electric field. The study was performed at different amplitudes of electric pulses, and the results were expressed by changes in the electrical properties of tissues evaluated by electrical impedance spectroscopy, current-voltage measurements, and by magnetic resonance imaging. Imaged were changes in water distribution and in the T_2 NMR relaxation times. The findings of our research provide useful insights and could be in support of an appropriate choice of electroporation assessment methods in relation to the food-matrix characteristics. This study was published in an article: Genovese Jessica, Kranjc Matej, Serša Igor, Petracci Massimiliano, Rocculi Pietro, Miklavčič Damijan, Mahnič-Kalamiza Samo. PEF-treated plant and animal tissues: insights by approaching with different electroporation assessment methods. *Innovative food science & emerging technologies*, ISSN 1466-8564, 2021, vol. 74, 102872, pp. 1-9, doi: 10.1016/j.ifset.2021.102872.

The research of our department has been supported by a number of international projects financed by the European Union. It was also supported within many bilateral projects and other scientific cooperations. In 2021, the department had cooperations with 131 partners from Slovenia and abroad. Among them were the following institutions that made the reported studies possible:

1. A.F. Ioffe Physico-Technical Institute, Saint Petersburg, Russia
2. AEROSOL razvoj in proizvodnja znanstvenih instrumentov d.o.o., Ljubljana, Slovenia
3. AMES d.o.o., Brezovica pri Ljubljani, Slovenia
4. ART REBEL 9 d.o.o., Ljubljana, Slovenia
5. Balder, d. o. o., Ljubljana, Slovenia
6. BASF, Heidelberg, Germany
7. Ben Gurion University, Beersheba, Israel
8. BIA SEPARATIONS d.o.o., Ajdovščina, Slovenia
9. BTT TEKSTIL d.o.o., Zgornja Kungota, Slovenia
10. Centre national de la recherché scientifique, Laboratoire de Spectrochimie Infrarouge et Raman, Thiais, France
11. Centre national de la recherché scientifique, Laboratory de Marseille, Marseille, France
12. Chalmers University of Technology, Physics Department, Gothenburg, Sweden
13. Clarendon Laboratory, Oxford, Great Britain
14. CosyLab d.d., Ljubljana, Slovenia
15. Department of Chemistry, College of Humanities and Sciences, Nihon University, Tokyo, Japan
16. Deutsches Elektronen-Synchrotron, Hamburg, Germany
17. Deutsches Krebsforschungszentrum, Heidelberg, Germany
18. École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
19. Eidgenössische Technische Hochschule - ETH, Zürich, Switzerland
20. Elettra (Synchroton Light Laboratory), Basovizza, Italy
21. European Synchrotron Radiation Facility, Grenoble, France
22. Facultad de Ciencia y Technologia, Universidad del Pais Vasco UPV/EHU, Leioa, Spain
23. Faculty of Physics, Adam Mickiewicz University, Poznan, Poland
24. Florida State University, Florida, USA
25. Forschungszentrum Dresden Rossendorf, Dresden, Germany
26. Gunma National College of Technology, Maebashi, Japan
27. Helmholtz-Zentrum Dresden-Rossendorf e.V., Dresden, Germany
28. High Magnetic Field Laboratory, Nijmegen, the Netherlands
29. High Magnetic Field Laboratory, Tallahassee, Florida, USA
30. High-Magnetic-Field Laboratory, Grenoble, France
31. Humboldt Universität Berlin, Institut für Biologie/Biophysik, Berlin, Germany
32. Illie Murguescu Institute of Physical Chemistry of the Romanian Academy, Bucharest, Romania
33. Infineon Technologies Austria AG, Vienna, Austria
34. Infinite d.o.o., Limbuš, Slovenia
35. Institut für Biophysik und nanosystemforschung OAW, Graz, Austria
36. Institut für Experimentalphysik der Universität Wien, Vienna, Austria
37. Institut Ruđer Bošković, Zagreb, Croatia
38. Institute of Biophysics at the Faculty of Medicine, University of Ljubljana, Ljubljana, Slovenia
39. Institute of Crystallography, Moscow, Russia
40. Institute of Theoretical Physics, Göttingen, Germany

41. Institute of Electronic Materials Technology, Warsaw, Poland
42. Institute of Molecular Physics, Polish Academy of Sciences, Poznan, Poland
43. Instituto Superior Tecnico, Departamento de Fisica, Lisbon, Portugal
44. Instrumentation Technologies, d. d., Solkan, Slovenia
45. International Center for Theoretical Physics, Trieste, Italy
46. International Human Frontier Science Program Organisation, Strasbourg, France
47. ISIS, Rutherford Appleton Laboratory, Didcot, Great Britain
48. Kavli Institute for Theoretical Physics, Santa Barbara, USA
49. Kimberly Clark, Atlanta, USA
50. King's College, London, Great Britain
51. University Medical Center Ljubljana, Ljubljana, Slovenia
52. KMZ Zalar Miran s.p., CNC obdelava kovin in drugih materialov, Ljubljana, Slovenia
53. Korea Basic Science Institute, Daejeon, South Korea
54. Krka, tovarna zdravil, d.d., Novo mesto, Slovenia
55. KTH Royal Institute of Technology, Stockholm, Sweden
56. Kyung Hee University of Suwon, Impedance Imaging Research Center, Seoul, South Korea
57. L'Oreal, Paris, France
58. Lek farmacevtska družba d.d., Ljubljana, Slovenia
59. Liquid Crystal Institute, Kent, Ohio, USA
60. Lotrič Certificiranje d.o.o., Železniki, Slovenia
61. LPKF LASER & ELECTRONICS d.o.o., Naklo, Slovenia
62. LVL livarstvo in orodjarstvo d.o.o., Kranj, Slovenia
63. Max Planck Institut, Dresden, Germany
64. Mayo Clinic, Rochester, Minnesota, USA
65. Melamin kemična tovarna d.d., Kočevje, Slovenia
66. Merck KGaA, Darmstadt, Germany
67. Metalurško-kemična industrija Celje, d.d., Celje, Slovenia
68. MH Hannover, Hannover, Germany
69. Ministry of Defense of the Republic of Slovenia, Ljubljana, Slovenia
70. Nanotul d.o.o., Ljubljana, Slovenia
71. National Academy of Sciences of Ukraine, Institute of Physics, Kyiv, Ukraine
72. National Center for Scientific Research "Demokritos", Aghia Paraskevi Attikis, Greece
73. National Institute for Research in Inorganic materials, Tsukuba, Japan
74. Vinča Nuclear Research Institute, Belgrade, Serbia
75. Optotek d. o. o., Ljubljana, Tsukuba
76. Oxford University, Department of Physics, Department of Materials, Oxford, Great Britain
77. PAB Akrapović, Buzet, Croatia
78. Paul Scherrer Institut, Villigen, Switzerland
79. Politecnico di Torino, Dipartimento di Fisica, Torino, Italy
80. Radbound University Nijmegen, Research Institute for Materials, Nijmegen, the Netherlands
81. RLS Merilna tehnika d. o. o., Žeja pri Komendi, Slovenia
82. Rwth Aachen University, Aachen, Germany
83. School of Physics, Hyderabad, Andhra Prades, India
84. SISSA, Trieste, Italy
85. SRC sistemske integracije d.o.o., Ljubljana, Slovenia
86. State College, Pennsylvania, USA
87. Stelar, Mede, Italy
88. The Faculty of Medicine of the University of Rijeka, Rijeka, Croatia
89. Institute of Physics, Zagreb, Croatia
90. TDK Electronics GmbH & Co OG, Deutschlandsberg, Austria
91. Technical University of Catalonia, Barcelona, Spain
92. TU Wien, Vienna, Austria
93. TELA merilni sistemi d.o.o., Ljubljana, Slovenia
94. The Geisel School of Medicine at Dartmouth, Hanover, USA
95. The Max Delbrück Center for Molecular Medicine in Berlin, Berlin, Germany
96. Tohoku University, Sendai, Japan
97. Tokyo University, Bunkjo, Tokyo, Japan
98. UNCOSS, Brussels, Belgium
99. Universita di Pisa, Dipartimento di Chimica e Chimica Industriale, Pisa, Italy
100. Universität Freiburg, Institut für Makromolekulare Chemie, Freiburg, Germany
101. Universität Mainz, Geowissenschaften, Mainz, Germany
102. Universität Regensburg, Regensburg, Germany
103. Université de la Méditerranée, Marseille, France
104. Université de Nice, Nice, France
105. Université de Picardie Jules Verne, Amiens, France
106. Université Paris Sud, Paris, France
107. University of Aveiro, Aveiro, Portugal
108. University of Bristol, Bristol, Great Britain
109. University of California at Irvine, Beckman Laster Institute and Medical Clinic, Irvine, California, USA
110. University of Duisburg, Duisburg, Germany
111. University of Durham, Durham, Great Britain
112. University of Innsbruck, Innsbruck, Austria
113. University of Leeds, Leeds, Great Britain
114. University of Linz, Institute of Chemistry, Department of Physical Chemistry & Linz Institute of Organic Solar Cells, Linz, Austria
115. University of Loughborough, Loughborough, Great Britain
116. University of Provence, Marseille, France
117. University of Tsukuba, Tsukuba, Ibaraki, Japan
118. University of Utah, Department of Physics, Salt Lake City, Utah, USA
119. University of Waterloo, Department of Physics, Waterloo, Ontario, Canada
120. University of Zürich, Zürich, Switzerland
121. University of Maribor, Maribor, Slovenia
122. University of Mons, Mons, Belgium
123. University of Munich and MPQ, Munich, Germany
124. University of Pavia, Pavia, Italy
125. University of North Carolina, Chapel Hill, USA
126. University of Wisconsin, Madison, USA
127. Wagenigen University, Laboratory of Biophysics, Wageningen, the Netherlands
128. Weizman Institute, Rehovot, Israel
129. Yonsei University, Seoul, South Korea
130. Blood Transfusion Centre of Slovenia, Ljubljana, Slovenia
131. Železarna Ravne, Ravne na Koroškem, Slovenia

ERC projects

1. H2020 - Cell-Lasers; Intracellular Lasers: Coupling of Optical Resonances with Biological Processes
   Asst. Prof. Matjaž Humar
   European Commission
2. H2020 - LOGOS; Light-Operated Logic Circuits from Photonic Soft-Matter
   Prof. Igor Muševič
   European Commission

Some outstanding publications in 2021

1. Schymura, Stefan, Drev, Sandra, Podlipec, Rok, Rijavec, Tomaž, Lapanje, Aleš, Štrok, Marko, et al. Dissolutionbased uptake of nanoparticles by freshwater shrimp: a dual-radiolabelling study of the fate of anthropogenic cerium in water organisms. Environmental science, Nano, ISSN 2051-8161, 11 pp., doi: 10.1039/d1en00264c.
2. Everts, J. C., Ravnik, M., Ionically charged topological defects in nematic fluids. *Phys. Rev. X,* 2021, **11**, 011054
3. Papič, M., Mur, U., Zuhail, K. P., Ravnik, M., Muševič, I., Humar, M., Topological liquid crystal superstructures as structured light lasers. *Proc. Natl. Acad. Sci. U.S.A.,* 2021, **118**, e2110839118
4. Peddireddy, K., Čopar, S., Le, V.K., Muševič, I., Bahr, C., Jampani, V.S.R., Self-shaping liquid crystal droplets by balancing bulk elasticity and interfacial tension. *Proc. Natl. Acad. Sci. U.S.A.,* 2021, **118**, e2011174118, 7
5. Pirker, L., Pogačnik Krajnc, A., Malec, J., Radulović, V., Gradišek, A., Jelen, A., Remškar, M., Mekjavić, I. B., Kovač, J., Mozetič, M., Snoj, L. Sterilization of polypropylene membranes of facepiece respirators by ionizing radiation. *J. Membr. Sci.* 2021, **619**, 118756
6. Del Pupo, S., Zupanič, E., et al. Tuning graphene doping by carbon monoxide intercalation at the Ni(111) interface. *Carbon*, 2021, **176**, 253.
7. Nasour, B., Vilfan, A., Golestanian, R., Minimum dissipation theorem for microswimmers. *Phys. Rev. Lett.*, 2021, **126**, 034503
8. Hickey, D., Vilfan, A., Golestanian, R., Ciliary chemosensitivity is enhanced by cilium geometry and motility. *eLife*, 2021, **10**, e66322
9. M. Klanjšek, „Singlets singled out", *Nature Physics* **17**, 1081 (2021).
10. X. Chen, T. Yang, Q. Zhang, L. Q. Chen, **V. Bobnar**, C. Rahn, Q. M. Zhang, Topological structure enhanced nanostructure of high temperature polymer exhibiting more than ten times enhancement of dipolar response, *Nano Energy* **88**, 106226 (2021).
11. Y. Tanama et al., "Robust coherent spin centers from stable azafullerene radicals entrapped in cycloparaphenylene rings", *Nanoscale* **13**, 19946-19955 (2021).

Some outstanding publications in 2020

1. T. Arh, M. Gomilšek, P. Prelovšek, M. Pregelj, M. Klanjšek, A. Ozarowski, S. J. Clark, T. Lancaster, W. Sun, J.-X. Mi, A. Zorko. *Origin of magnetic ordering in a structurally perfect quantum kagome antiferromagnet*. Phys. Rev. Lett. **125** (2020) 027203.
2. P. Khuntia, M. Velazquez, Q. Barthélemy, F. Bert, E. Kermarrec, A. Legros, B. Bernu, L. Messio, A. Zorko, P. Mendels"Gapless ground state in the archetypal quantum kagome antiferromagnet ZnCu3(OH)6Cl2", Nat. Phys. 16, 469 (2020).
3. A. J. Hess, G. Poy, Jung-Shen B. Tai, S. Žumer, I. I. Smalyukh. *Control of light by topological solitons in soft chiral birefringent media.* Phys. Rev. X **10** (2020) 031042.
4. G. Poy, A. J. Hess, I. I. Smalyukh, S. Žumer. *Chirality-Enhanced Periodic Self-Focusing of Light in Soft Birefringent Media.* Phys. Rev. Lett. **125** (2020) 077801.
5. T. Strübing, A. Khosravanizadeh, A. Vilfan, E. Bodenschatz, R. Golestanian, I. Guido. *Wrinkling Instability in 3D Active Nematics*. Nano Lett. **20** (2020) 6281–6288.
6. J. Binysh, Ž. Kos, S. Čopar, M. Ravnik, G. P. Alexander. *Three-Dimensional Active Defect Loops.* Phys. Rev. Lett. **124** (2020) 088001.
7. K. Pal, A. Si, G. S. El-Sayyad, M. A. Elkodous, R. Kumar, A. I. El-Batal, S. Kralj, S. Thomas. *Cutting edge development on graphene derivatives modified by liquid crystal and CdS/TiO$_2$ hybrid matrix: optoelectronics and biotechnological aspects.* Critical Reviews in Solid State and Materials Sciences (2020).

8. H. Massana-Cid, A. Ortiz-Ambriz, A.Vilfan, P. Tierno. *Emergent collective colloidal currents generated via exchange dynamics in a broken dimer state*, Sci. Adv. **6** (2020) eaaz2257.

9. D. Richter, M. Marinčič, M. Humar. *Optical-resonance-assisted generation of super monodisperse microdroplets and microbeads with nanometer precision*. Lab Chip **20** (2020) 734–74.

10. P. Campinho, P. Lamperti, F. Boselli, A. Vilfan, J. Vermot. *Blood Flow Limits Endothelial Cell Extrusion in the Zebrafish Dorsal Aorta*. Cell Reports **31** (2020) 107505.

11. L. Pirker, B. Višić, S. D. Škapin, G. Dražić, J. Kovača, M. Remškar. *Multi-stoichiometric quasi-two-dimensional W_nO_{3n-1} tungsten oxides.* Nanoscale **12** (2020) 15102–15114.

12. A. Hassanien, B. Zhou, A. Kobayashi. *Spontaneous Antiferromagnetic Ordering in a Single Layer of $(BETS)_2GaCl_4$ Organic Superconductor.* Advanced Electronic Materials **6** (2020).

13. H. Kokot, B. Kokot, A. Sebastijanović, R. Podlipec, A. Krišelj, P. Čotar, M. Pušnik, P. Umek, S. Pajk, I. Urbančič, T. Koklič, J. Štrancar, et al. *Prediction of chronic inflammation for inhaled particles: the impact of material cycling and quarantining in the lung epithelium*. Adv. Mater. **32** (2020) 2003913.

14. A. Barbotin, I. Urbančič, S. Galiani, C. Eggeling, M. J. Booth. *Background reduction in sted-fcs using a bi-vortex phase mask*. ACS Photonics **7** (2020) 1742–1753.

15. A. Frawley, V. Wycisk, Y. Xiong, S. Galiani, E. Sezgin, I. Urbančič, A. Vargas Jentzsch, K. G. Leslie, C. Eggeling, H. L. Anderson. *Super-resolution resolft microscopy of lipid bilayers using a fluorophore-switch dyad.* Chem. Sci. **11** (2020) 8955–8960.

Awards and Appointments

1. Dr Luka Drinovec and Prof Griša Močnik, PhD: The Puh Award for outstanding achievements in the development of methods for measuring aerosol absorption, Ljubljana, The Government of the Republic of Slovenia

2. Asst. Prof. Anton Gradišek: Award for the best oral presentation at Ecobalt 2021 with the title "Particle Removal Efficiency of Face Masks During the Covid-19 Pandemic", Riga, Latvia (virtual)

3. Asst. Prof. Anton Gradišek: Team JSI vs COVID won 2nd place at XPRIZE Pandemic Response Challenge for finding best strategies against covid, Culver City, California, USA, XPRIZE Foundation (virtual)

4. Prof Miha Ravnik, PhD: The Blinc Award for physicists at the beginning of their career, Ljubljana, Faculty of Mathematics and Physics and Jožef Stefan Institute

5. Aljaž Kavčič, M.Sc.Phys.: The Prešeren Award for his master's thesis "Microscopy and sensing through scattering tissues using optical microresonators" (mentor Asst. Prof. Matjaž Humar), Ljubljana, University of Ljubljana

6. Prof Samo Kralj, PhD: Award for outstanding achievements in higher education, Ljubljana, The Council for Higher Education of the Republic of Slovenia

7. Asst. Prof. Uroš Tkalec: The Blinc Award for extraordinary one-time achievement in physics for a research in the field of imbalanced complex fluids that was published in *Nature Communications*, Ljubljana, Faculty of mathematics and physics and Jožef Stefan Institute

Organization of conferences, congresses and meetings

1. Alpine NMR Workshop, Bled, 16–20 September 2021

Patents granted

1. Janez Štrancar, Rok Podlipec, Iztok Urbančič, Zoran Arsov, Andrej Vrečko, Image-processing apparatus and image-processing method for detection of irregularities in tissue, EP3755994 (B1), European Patent Office, 26. 05. 2021.

2. Gregor Filipič, Kristina Eleršič, Darij Kreuh, Janez Kovač, Uroš Cvelbar, Miran Mozetič, A method of colouring titanium and titanium alloys, GB2530805 (B), Intellectual Property Office, 24. 11. 2021.

3. Vid Bobnar, Barbara Malič, Aleksander Matavž, A method for producing polymeric surface modification layers, SI25887 (A), Slovenian Intellectual Property Office, 31. 03. 2021.

INTERNATIONAL PROJECTS

1. ERC H2020 - Cell-Lasers; Intracellular Lasers: Coupling of Optical Resonances with Biological Processes
   Asst. Prof. Matjaž Humar
   European Commission

2. ERC H2020 - LOGOS; Light-Operated Logic Circuits from Photonic Soft-Matter
   Prof. Igor Muševič
   European Commission

3. Measurements of the Thickness of Chromium Deposits on a Glass Surface
   Prof. Miha Škarabot
   Pab Akrapović d. o. o.

4. COST CA16109; Chemical On-Line Composition and Source Apportionment of Fine Aerosol

Prof. Griša Močnik
Cost Office
5. COST CA16218; Nanoscale Coherent Hybrid Devices for Superconducting Quantum Technologies
Dr. Abdelrahim Ibrahim Hassanien
Cost Association Aisbl
6. COST CA16221; Quantum Technologies with Ultra-Cold Atoms
Dr. Peter Jeglič
Cost Association Aisbl
7. COST CA17121; Correlated Multimodal Imaging in Life Sciences
Prof. Janez Štrancar
Cost Association Aisbl
8. COST CA17139; European Topology Interdisciplinary Action
Prof. Slobodan Žumer
Cost Association Aisbl
9. COST CA16202; International Network to Encourage the Use of Monitoring and Forecasting Dust Products
Prof. Griša Močnik
Cost Association Aisbl
10. COST CA9108 - HiSCALE; High-Temperature SuperConductivity for AcceLerating the Energy Transition
Dr. Abdelrahim Ibrahim Hassanien
Cost Association Aisbl
11. BIO-OPT-COMM; A Living Optically-Communicating Neural Network
Asst. Prof. Matjaž Humar
Hfspo- International Human Frontier
12. H2020 - ENGIMA; Engineering of Nanostructures with Giant Magneto-Piezoelectric and Multicaloric Functionalities
Prof. Zdravko Kutnjak
European Commission
13. H2020 - ATHENA; Implementing Gender Equality Plans to Unlock Research Potential of RPOs and RFOs in Europe
Prof. Maja Remškar
European Commission
14. H2020 - FoodTraNet; Advanced Research and Training Network in Food Quality, Safety and Security
Asst. Prof. Matjaž Humar
European Commission
15. H2020 - QMatCh; Towards Quantum States of Matter via Chemistry under Extreme Conditions
Prof. Denis Arčon
European Commission
16. Conservation of Cultural Heritage Indoors - The Case of Leonardo da Vinci's "Last Supper"
Prof. Griša Močnik
Slovenian Research Agency
17. Lipid Wrapped Nanoparticles and Activity of Factor Xa
Dr. Tilen Koklič
Slovenian Research Agency
18. Studies of Nanoporous Materials for Hydrogen Storage
Prof. Janez Dolinšek
Slovenian Research Agency
19. Magnetoresonance Study of Spin-Liquid Candidates
Prof. Andrej Zorko
Slovenian Research Agency
20. Advanced Organic and Inorganic Thin-Film Composites with Enhanced Dielectric and Electromechanical Response
Prof. Zdravko Kutnjak
Slovenian Research Agency
21. New Electronic States Emergent via Cross-Coupling between Magnetism and Electrical Conduction in Itinerant Antiferromagnetic Systems
Prof. Denis Arčon
Slovenian Research Agency
22. Hemoglobin-Based Nano-Spectral Non-Linear Imaging for Future Label-Free Medical Diagnostics
Dr. Rok Podlipec
Slovenian Research Agency
23. Impact of Fireworks on Air Pollution in Urban Environments
Asst. Prof. Anton Gradišek
Slovenian Research Agency
24. Investigation of Air Pollution with Nanoparticles Caused by Fireworks
Prof. Maja Remškar
Slovenian Research Agency
25. Positioning and Spatial Control of Magnetic Fullerides
Prof. Denis Arčon
Slovenian Research Agency
26. Tunable Memristive Switching in Carbon Nanotube Network for Neuromorphic Computing
Dr. Abdelrahim Ibrahim Hassanien
Slovenian Research Agency
27. Plasmon-Coupled Microcavities for Real-Time Molecular Sensing Inside Live Cells

Asst. Prof. Matjaž Humar
Slovenian Research Agency
28. Criticality Concept in Antiferroelectric Materials (CAMat)
Dr. Nikola Novak
Slovenian Research Agency

RESEARCH PROGRAMMES

1. Magnetic resonance and dielectric spectroscopy of „smart" new materials
Prof. Denis Arčon
2. Physics of Soft Matter, Surfaces and Nanostructures
Prof. Miha Ravnik
3. Experimental Biophysics of Complex Systems
Prof. Janez Štrancar

R & D GRANTS AND CONTRACTS

1. Electroporation-based treatments with new high-frequency electroporation pulses
Prof. Igor Serša
2. Reconstruction of electrical conductivity of tissues by means of magnetic resonance techniques
Prof. Igor Serša
3. Phase transitions towards coordination in multilayer networks
Dr. Uroš Jagodič
4. Development of building blocks for new European quantum communication network
Dr. Peter Jeglič
5. Development of high-performance piezoelectric coatings for self-powering of nonwovens used in e-mobility
Prof. Vid Bobnar
6. Probing spin states near the surface of quantum spin materials
Prof. Denis Arčon
7. Advanced soft nematocaloric materials
Asst. Prof. Brigita Rožič
8. Multicaloric cooling
Prof. Zdravko Kutnjak
9. Optimization of MRI techniques for assessment of thrombolytic treatment outcome
Prof. Igor Serša
10. Intracellular lasers: Coupling of optical resonances with biological processes
Asst. Prof. Matjaž Humar
11. Study of intracellular forces by deformable photonic droplets
Asst. Prof. Matjaž Humar
12. Electrocaloric elements for active cooling of electronic circuits
Prof. Vid Bobnar
13. Advanced inorganic and organic thin films with enhanced electrically-induced response
Prof. Vid Bobnar
14. Adverse outcome pathway leading to atherosclerosis
Dr. Tilen Koklič
15. Liquid-crystal microdroplet lasers for sensing inside live cells
Zuhail Kottoli Poyil
16. Stabilization and destabilisation of spin liquids by perturbations
Prof. Andrej Zorko
17. Physics of Majorana fermions in Kitaev magnets
Dr. Martin Klanjšek
18. Novel experimental approach for determination of quantum spin liquids
Prof. Andrej Zorko
19. Topological turbulence in confined chiral nematic fields
Prof. Miha Ravnik
20. Controllable broadband electromagnetic-radiation shielding
Dr. Matej Pregelj
21. Intelligent Content-Aware Nanospectroscopy (iCAN) of molecular events in nanoparticles-induced neurodegeneration
Asst. Prof. Iztok Urbančič
22. Self-assembly of Photon-Enabled Circuits using Topologically Reconfigurable Anisotropic Liquids
Venkata Subba Rao Jampani
23. Advanced optical magnetometry of vortices in unconventional superconductors
Prof. Denis Arčon
24. Diamond-assisted quantum processing of fullerene qubits
Prof. Denis Arčon
25. Coulombic subgap states in superconducting quantum devices
Prof. Denis Arčon
26. Spatial and temporal shaping of laser light for minimally invasive ophthalmic procedures
Prof. Janez Štrancar
27. Magnetic, electric and stress – field programming of shape response in polymer-dispersed liquid crystal elastomers – based actuators
Dr. Andraž Rešetič

28. Cryptographically secure random number generator
Dr. Peter Jeglič
29. Cryptographically secure random number generator
Dr. Peter Jeglič
Urad Vlade Republike Slovenije za varovanje tajnih podatkov
30. CROSSING - Crossing Borders and Scales - An Interdisciplinary Approach
Prof. Janez Štrancar
Helmholtz-Zentrum Dresden-rossendorf E.v.
31. International Alpine NMR Workshop
Prof. Igor Serša

NEW CONTRACTS

1. Detecion of Non-Anthropogenic Air Pollution project (DNAAP)
Prof. Griša Močnik
Aerosol d. o. o.
2. Magnetic, electric and stress - field programming of shape response in polymer-dispersed liquid crystal elastomers - based actuators
Dr. Andraž Rešetič
Kmz - Zalar Miran s.p.
3. Research and analysis of new molecular events and their causal connections in vitro
Prof. Janez Štrancar
Infinite d. o. o.

VISITORS FROM ABROAD

1. Dr Nych Andriy, National Academy of Sciences of Ukraine, Kyiv, Ukraine, 28 February–13 March 2021
2. Ivanović Arso, University of Montenegro, Podgorica, Montenegro, 1 March–20 April 2021
3. Dr Ryzhkova Anna, ASML B.V. Nederland, Amsterdam, The Netherlands, 30 May–19 June 2021
4. Dr Višić Bojana, Institute of Physics, Belgrade, Serbia, 31 May–1 August 2021
5. Dr Nych Andriy and Dr Ognysta Uliana, National Academy of Sciences of Ukraine, Kyiv, Ukraine, 18 June–1 August 2021
6. Dr Kimouche Amina, University of Potsdam, Potsdam, Germany, 25 June–27 August 2021
7. Šenjug Pavla, Faculty of Science, Zagreb, Croatia, 30 August–3 September 2021
8. Dr Sebastiao Pedro, Instituto Superior Tecnico, Lisbon, Portugal, 11–18 September 2021
9. Dr Buganski Ireneusz, AGH Krakow, Krakow, Poland, 15 September–15 November 2021
10. Tanuma Yuri, CRNS, Nantes, France, 5–13 October 2021
11. Dr Lukyanchuk Igor and Dr Razumnaya Anna, Université de Picardie Jules Verne, LPMC, Amiens, France, 15 October–7 November 2021
12. Wojciechowski Adam, University of Krakow, Krakow, Poland, 16–20 October 2021
13. Dr Vinokour Valerii, Consortium for Advanced Science and Engineering, Chicago, USA, 29 October–3 November 2021
14. Dragojević Rajko and Šćepanović Stefan, University of Montenegro, Podgorica, Montenegro, 1 November–1 December 2021
15. Volkmann Jannis, Justus-Liebig University, Giessen, Germany, 14–20 November 2021
16. Dr Anyfantakis Emmanouil, University of Luxembourg, Luxembourg, Luxembourg, 14–20 November 2021
17. Dr Višić Bojana, Institute of Physics, Beograd, Serbia, 6–18 December 2021
18. Prof. El Marssi Mimoun, Université de Picardie Jules Verne, LPMC, Amiens, France, 10–12 December 2021

STAFF

Researchers
1. Prof. Tomaž Apih
2. Prof. Denis Arčon*
3. Prof. Vid Bobnar
4. Prof. Janez Dolinšek*
5. Dr. Gregor Filipič
6. Asst. Prof. Anton Gradišek
7. Dr. Alan Gregorovič
8. Abdelrahim Ibrahim Hassanien, B. Sc.
9. Asst. Prof. Matjaž Humar
10. Dr. Venkata Subba Rao Jampani
11. Dr. Peter Jeglič
12. Dr. Andreja Jelen
13. Dr. Marjan Ješelnik*
14. Dr. Martin Klanjšek
15. Dr. Tilen Koklič
16. Dr. Georgios Kordogiannis
17. Prof. Samo Kralj*
18. Prof. Zdravko Kutnjak
19. Dr. Mojca Urška Mikac
20. Prof. Griša Močnik*
21. Asst. Prof. Aleš Mohorič*
22. **Prof. Igor Muševič*, Head**
23. Dr. Nikola Novak
24. Dr. Andriy Nych
25. Asst. Prof. Dušan Ponikvar*
26. Dr. Matej Pregelj
27. Dr. Amid Ranjkesh Siahkal
28. Prof. Miha Ravnik*
29. Prof. Maja Remškar
30. Asst. Prof. Brigita Rožič
31. Prof. Igor Serša
32. Prof. Miha Škarabot
33. Prof. Janez Štrancar
34. Asst. Prof. Uroš Tkalec*
35. Dr. Polona Umek
36. Dr. Iztok Urbančič
37. Dr. Herman Josef Petrus Van Midden
38. Dr. Mahendran Vellaichamy
39. Asst. Prof. Andrej Vilfan
40. Dr. Stanislav Vrtnik
41. Prof. Aleksander Zidanšek
42. Prof. Andrej Zorko
43. Dr. Erik Zupanič
44. Prof. Slobodan Žumer

Postdoctoral associates
45. Dr. Matej Bobnar
46. Dr. Maja Garvas
47. Dr. Matjaž Gomilšek
48. *Dr. Urška Gradišar Centa, left 15.10.21*
49. Dr. Uroš Jagodič*
50. *Dr. Zuhail Kottoli Poyil, on leave since 01.04.21*
51. Dr. Primož Koželj
52. *Dr. Mitja Krnel, on leave 07.04.21*
53. Dr. Marta Lavrič
54. Dr. Jože Luzar
55. Dr. Deepshika Malkar
56. Dr. Maruša Mur
57. Dr. Luka Pirker
58. Dr. Rok Podlipec
59. *Dr. Gregor Posnjak, on leave since 01.08.19*
60. Dr. Andraž Rešetič
61. Dr. Anna Ryzhkova
62. *Dr. Saide Umerova, left 28.08.21*
63. Dr. Jernej Vidmar*
64. Dr. Bojana Višić

Postgraduates
65. Tina Arh, B. Sc.
66. Dejvid Črešnar, B. Sc.
67. Nikita Derets, B. Sc.
68. Darja Gačnik, B. Sc.
69. Žiga Gosar, B. Sc.
70. Katja Gosar, B. Sc.
71. *Dr. Saša Harkai, left 01.12.21*
72. Anton Hromov, M. Sc.
73. *Nejc Janša, M. Sc., left 01.11.21*
74. Vida Jurečič, B. Sc.
75. Aljaž Kavčič, B. Sc.
76. Hana Kokot, B. Sc.
77. Boštjan Kokot, B. Sc.
78. Matjaž Malok, B. Sc.
79. Bojan Marin*, M. Sc.
80. Matevž Marinčič, B. Sc.
81. *Dr. Aleksander Matavž, on leave since 19.01.20*
82. Tadej Mežnaršič, B. Sc.
83. Matic Morgan, B. Sc.
84. Arkalekha Neogi, M. Sc.
85. Rok Peklar, B. Sc.

86. Gregor Pirnat, B. Sc.
87. Jaka Pišljar, B. Sc.
88. Anja Pogačnik Krajnc, B. Sc.
89. Aleksandar Sebastijanović, B. Sc.
90. Linsy Jane Selvin Robert, M. Sc.
91. *Dr. Marion Antonia Van Midden, on leave since 01.09.21*
92. Rebeka Viltužnik, B. Sc.

Technical officers
93. Petra Čotar, B. Sc.
94. Dr. Luka Drinovec*
95. Maša Kavčič, B. Sc.
96. Ana Krišelj, B. Sc.
97. Ivan Kvasić, B. Sc.
98. Blaž Mencinger, M. Sc.
99. Jaka Močivnik, B. Sc.

Technical and administrative staff
100. Dražen Ivanov
101. Janez Jelenc, B. Sc.
102. Davorin Kotnik
103. Vesna Lopatič, B. Sc.
104. Silvano Mendizza
105. Peter Mihor
106. Janja Milivojević
107. Ana Sepe, B. Sc.
108. Marjetka Tršinar

Note:
* part-time JSI member

BIBLIOGRAPHY

ORIGINAL ARTICLE

1. Neelakandan Marath Santhosh, Kush K. Updhyay, Petra Stražar, Gregor Filipič, Janez Zavašnik, André Mão de Ferro, Rui Pedro Silva, Elena Tatarova, Maria de Fátima Montemor, Uroš Cvelbar, "Advanced carbon-nickel sulfide hybrid nanostructures: extending the limits of battery-type electrodes for redox-based supercapacitor applications", *ACS applied materials & interfaces*, 2021, **13**, 17, 20559–20572.

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LABORATORY OF GASEOUS ELECTRONICS

F-6

The research activities within the Department of Gaseous Electronics cover various research areas, ranging from the science of gases and gaseous discharges, plasma nanoscience, plasma biology and biomedicine, advanced sensors, surface electronics and crystals to advanced vacuum science and technology. Within this scope, we are exploring different gaseous and plasma systems and their use in various fields important for the progress of humanity. The research activities are, therefore, quite diverse. The most important achievements and progress beyond the existing state of the art are communicated in the paragraphs below.

Head:
Prof. Uroš Cvelbar

The major activities of the department encompass interconnected fields of research such as the science of gases and gaseous discharges, plasma nanoscience, processing and synthesis of nanomaterials, plasma chemistry, plasma electrochemistry and catalysis, plasma biomedicine and biotechnology, gas sensors, research on field emission from nanostructured materials, optoelectronics, vacuum science, design of vacuum systems, vacuum thermal insulation and other emerging topics relevant to the manipulation of atoms and electrons. These topics of research are brought together to solve different problems and tackle grand challenges in science and technology as well as to support new emerging fields of research.

New partner cooperation with the Max Planck Institute. In July 2021 the Max Planck Society began to fund a Slovenian-German partner research group involving the JSI and Max Planck Institute for Iron Research (MPIE), Düsseldorf, Germany. The partner research on the topic of high-performance materials aims to advance the resistance of the materials exposed simultaneously to gas loading and high temperatures and to unravel the role of the microstructure evolution and its influence on the gas-solid interaction. The partner group funded for the next five years is led by doc. dr. Zavašnik from F6 and established at the MPIE, at the department Structure and Nano-/Micromechanics of Materials (https://www.mpie.de/4580830/new-partner-group-on-high-performance-materials).

Atmospheric pressure plasma research and a breakthrough in the stabilisation of liquid instabilities. In physics, liquid instabilities such as vortices, oscillatory motions, turbulent flows, etc., also known under names such as the Kelvin-Helmholtz instability, Plateau-Rayleigh instability, Rayleigh-Taylor instability, etc., have been the paramount problem of fluid dynamics for decades. Surprisingly, little effort has been taken to address these instabilities, especially at the gas-liquid interphases, beyond mere redesigns of the geometric gas-blowing systems to reduce or mitigate these instabilities, especially during the relevant processes of manufacturing. Now, an international team composed of KFE, KAIST and our department from the Jožef Stefan Institute made a significant breakthrough in the field by finding that a simple use of ionised gas generated by plasma discharge at atmospheric pressure can stabilise such liquids without the standard redesign of the gas-blowing system. Therefore, we managed to alternate the blown-gas jet properties by simply changing the properties of the jet by discharging the blown gas, which resulted in completely new properties and new jet behaviour of the interacting liquid surfaces.

Such gas discharges have been known for decades. They are known as cold atmospheric pressure plasmas, characteristically generated by gas jets or at discharging surfaces. Different gas mixtures including some inert gases (like argon or helium) are used or, simply, ambient air can be used in these discharges. It is characteristic of these plasmas that the temperature is rather low so that the gas is reasonably cold, almost at room temperature or not significantly hotter than tens of degrees Celsius. However, such plasmas also contain a host of other species, including particles like electrons, ions, etc., which can have a much higher temperature, creating a thermodynamically non-equilibrium system.

When these particles interact with other outside particles or, better, molecules, an interesting phenomenon arises, known as an electric wind. This wind is induced by the momentum transfer from accelerated charged species to the neutral gas under an electric field, also resulting in the generation of an electrohydrodynamic force. We already reported on this phenomenon in *Nature Communications* (9 (2018) 371).

We applied this phenomenon to the gas-liquid interphase to successfully solve the overarching problem of fluid dynamic instabilities, as described above. The most important cornerstone of our concept was the exploitation of the generated electrohydrodynamic force exerted towards the liquid surface, which resulted in the stabilisation of the unstable liquid structures, as shown in gas cavities. This stabilisation was done with a weakly ionised gas jet consisting of pulsed ionisation waves, a gas discharge type often called plasma

Figure 1: Cavity (or dimple) formation at the water surfaces subjected to a neutral helium-gas jet (left) and a weakly ionized helium-gas jet (right)
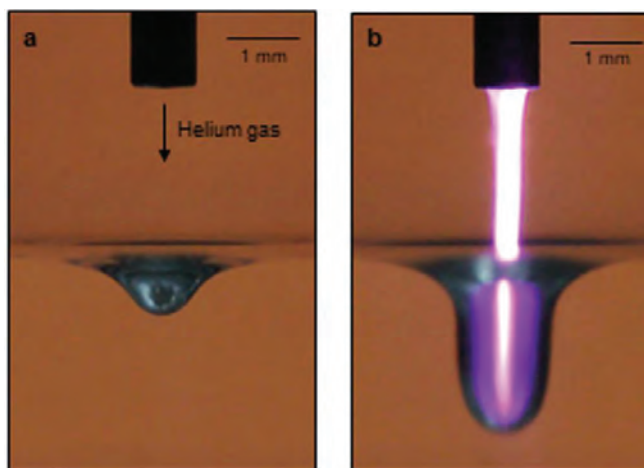
Figure 2: Water surface deformation by neutral (a) and ionized (b) helium-gas jets
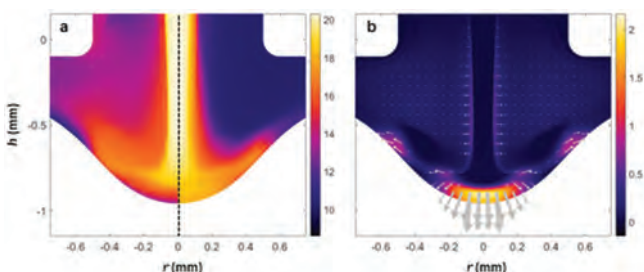

Figure 3: Theoretically estimated plasma characteristics; the space charge density (a) and electrohydrodynamic force (b)

Figure 4: Procedure for the generation of plasma activated water and viral inactivation

bullets where the force was exerted via the electrohydrodynamic flow on the water surface. As a result, a dimpled cavity was expended without destabilisation. Furthermore, both the bidirectional electrohydrodynamic gas flow and electric field parallel to the gas-water interface and interacting within the cavity, created a more stable liquid surface. We experimentally and numerically demonstrated that the electrohydrodynamic force generated inside the formed cavity causes a cavity extension while maintaining stability, despite the critical gas-flow rate being on the verge of unstable oscillatory motion. These results were a crucial breakthrough step towards understanding the interaction of plasma with liquid surfaces and its stabilisation. The results were published in *Nature* (592 (2021) 49-53).

Awarded 2021 results for atmospheric pressure plasmas used in decontamination processes. The members of department F6 uncovered new insights into the areas of global significance, including water security and airborne virus control, generating high-impact scientific results with the potential to stimulate enormous socioeconomic benefit in Slovenia and beyond. The team won a national accolade for their work on mycotoxin contamination presented in the *Journal of Hazardous Materials* (Hojnik *et al.* JHM, 2021), received the award for scientific excellence in the field of biotechnology, while their paper published in *Plasma Processes and Polymers* (Hojnik et al., 2021) was recognised as one of the most cited papers of the year.

Aerosolised plasma activated water for large-area viral decontamination. Novel and efficient surface-disinfection techniques are urgently needed to minimize the spread of infectious viral agents such as SARS-CoV-2. The members of F6 studied the effect of nebulized plasma activated water (nPAW) on MS2 bacteriophages, used as a surrogate for pathogenic viruses such as SARS-CoV-2. Bacteriophages were deposited on four different test materials that are commonly found in a healthcare setting and the efficiency of nPAW was assessed and compared against hydrogen peroxide (Figure 4). It was demonstrated that nPAW successfully inactivated MS2 on non-porous surfaces (glass, polypropylene and stainless steel), while being ineffective against MS2 deposited on fabric. The efficacy of nPAW was impacted by the distance of the test material from the nebulizer output, test material coverage and the influence of interfering organic substances, such as saliva. For non-porous materials, the surface finish played the key role in providing the inactivation efficacy of the approach. Ultimately, it was demonstrated that nebulization of plasma activated water was sufficient to successfully eliminate >99.999% of the viral load deposited on all non-porous tested surfaces, an efficiency that compares well against common chemical disinfectants such as hydrogen peroxide. The study highlights the potential of nPAW as an efficient and convenient surface decontamination technology and was submitted for publication in the high-impact journal *ACS Environmental Science & Technology*.
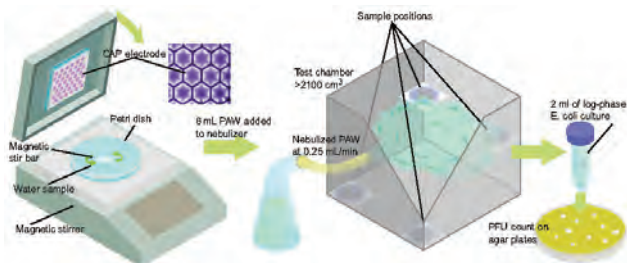
Low-temperature plasma for the degradation of micropollutants. Developing novel, fast and efficient, ecologically benign processes for removing organic contaminants is crucial for sustainable water treatment. For this reason, the members of F6, in collaboration with the colleagues from department O2, explored the implementation of Cold Atmospheric pressure Plasma (CAP) generated in ambient air as an efficient agent for the removal of bisphenol A (BPA) and bisphenol S (BPS), known as endocrine disrupting compounds in water and wastewater (Figure 3), by monitoring degradation kinetics and its transformation products.

Using advanced LC-MS/MS it was determined that the highest removal efficiencies of BPA (>98%) and BPS (>70%) were obtained after 480 s of CAP exposure. Pseudo-first-order kinetics revealed that BPA ($-k_t = 0.0044$–0.0090 s^{-1}) degrades faster than BPS ($-k_t = 0.0004$–0.0023 s^{-1}) and that the degradation is also time- and CAP power-dependent, while the initial concentration or matrix type had a negligible effect. This study also tentatively identified three previously reported products and one novel transformation product of BPA and four novel transformation products of BPS. Their postulated structures suggested similar breakdown mechanisms, i.e., hydroxylation followed by ring cleavage. The results demonstrate that the CAP technology is an effective process for the degradation of both BPA and BPS without the need for additional chemicals, indicating it is a highly promising method for water

and wastewater remediation and has been submitted for publication in the high-impact journal *Science of the Total Environment.*

Plasma design of nanoplasmonic sensors for bio-chemical sensing applications. In the frame of this research, the members of F6 designed highly efficient nanocarbon-based optical sensors via plasma nanosynthesis for biohazard detection. Mycotoxins are widespread toxic entities in the agriculture and food industries that can induce cancer growth and immune deficiency, posing a serious health threat for humankind. These hazardous compounds are produced naturally by various moulds (fungi) that contaminate different food products and can be detected in cereals, nuts, spices and other food products. However, their detection, especially at minimally harmful concentrations, remains a serious analytical challenge. This research shows that high-performing plasmonic substrates (analytical enhancement factor = 5×10^7) based on plasma-grown vertical hollow carbon nanotubes can be applied for immediate detection of the most toxic mycotoxins. Due to excellent sensitivity, allowing the operation at ppb concentrations, it is possible to collect vibrational fingerprints of aflatoxin B1, zearalenone, alternariol and fumonisin B1, and highlight the key spectral differences between them using the principal component analysis. Compared to the time-consuming conventional methods, including thin-layer chromatography, gas chromatography, high-performance liquid chromatography and enzyme-linked immunosorbent assay, the designed surface-enhanced Raman spectroscopy substrates provide a clear roadmap to reducing the detection time-scale of mycotoxins down to seconds.

Photonic techniques based on evanescent wave sensing, such as the method using plasmonic and nanostructured metallic/semiconductor materials, hold significant potential in biosensing and the associated analysis of biomolecular interactions. Our research of nanoplasmonic sensors led to advances in the optical response of the surface plasmon resonance (SPR) based sensor by improving the electric-field penetration depth. However, the conventional SPR suffers from low penetration depths (<300 nm), limiting the applications for surface interactions and the analysis of larger biomolecules, such as bacterial cells with a typical size of ~1 μm. These cases result in the measured signal being non-monotonic with the concentration, making the technique unreliable for high concentrations. Infrared wavelengths can be used, but then the signal contrast suffers, and the instruments required for mid-infrared or longer wavelengths are prohibitively expensive. Based on this, we developed a "nearly" guided SPR (NGWSPR) structure to enhance the performance of these sensors by increasing the penetration depth and figure of merit using the wavelengths in the optical telecommunication window where off-the-shelf instruments are available at low costs. The use of this technique for monotonic detection of cultured live *Escherichia coli* bacterial cells was demonstrated, thus opening a pathway to the utilization and promottion of biosensing, biomedical research and industrial applications.

Lastly, we prepared a comprehensive overview of plasmonic-based sensors used in viral diagnostics. Early diagnosis of viral infection and disease control have always been critical. Virus detection can be achieved based on various plasmonic phenomena, including propagating surface plasmon resonance (SPR), localized SPR, surface-enhanced Raman scattering, surface-enhanced fluorescence and surface-enhanced infrared absorption spectroscopy. The present review covers all available information on the plasmonic-based virus detection and collected data on these sensors, based on several parameters. This data will assist us in advancing the research and development of a new generation of versatile virus biosensors and it was presented in a high-profile article in Nature *Communication Biology*.

Plasma for sustainable packaging with cellulose. Cellulose-based products are gaining increased interest, especially as a top-choice material for replacing plastics in packaging-related fields. Nevertheless, a high inherent wettability often hinders its advancement in becoming an efficient substitute
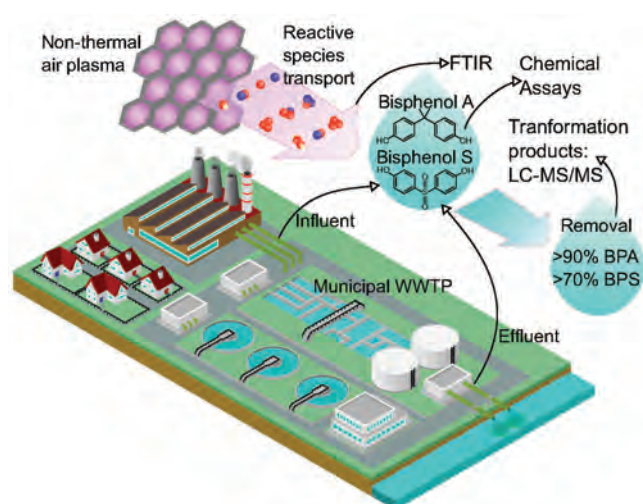

Figure 5: Concept for the plasma mediated degradation of BPA and BPS in real wastewater samples
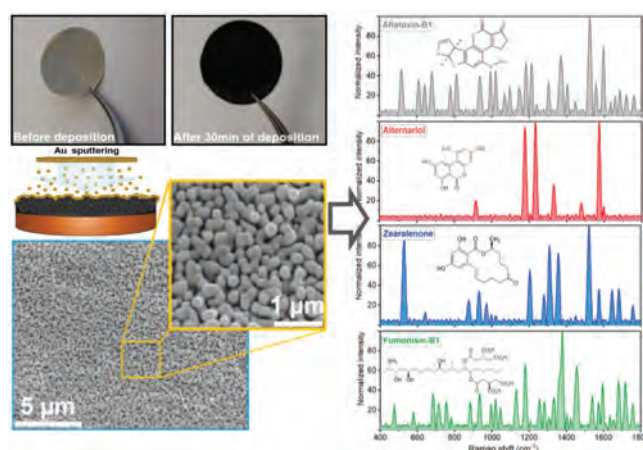

Figure 6: Plasma-made gold-decorated multiwall nanotubes designed for the Raman sensing of cancerogenic mycotoxins, presented in Small
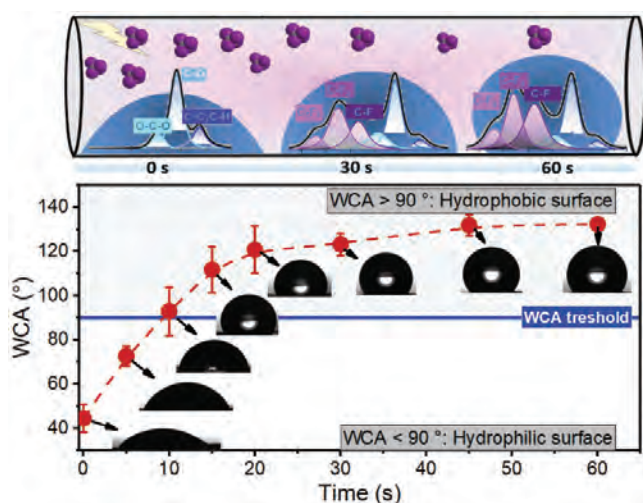

Figure 7: Plasma-induced hydrophilic to hydrophobic conversion of cellulose nanofibrils

in the packaging industry. To overcome this challenge, fluorocarbon plasma processing was implemented for the improvement of cellulose surface hydrophobicity. This was done on nanofibril films exposed to CF_4 plasma in order to achieve a hydrophilic-to-hydrophobic conversion in less than 10s. The saturation of the water contact angle (approximately 130±5°) was obtained after only 30s of plasma processing. The surface fluorination was the result of newly formed $C–F_3$, $C–F_2$ and C–F bonds, confirmed by high-resolution C 1s XPS spectra. A prolonged continuous plasma functionalization resulted in structural vibrational alterations associated mostly with the intense IR and Raman active stretching $C–F_2$ mode. Simultaneously, ATR-FTIR revealed the formation of a surface-linked IR active H–F functional group. Our findings successfully demonstrate that CF_4 plasma processing can be an effective way for an ultrafast cellulose conversion from a hydrophilic to hydrophobic surface, achieved within seconds due to plasma-created water-repellent surface functional groups.

Fusion research and understanding the interactions of hydrogen isotopes with fusion-related materials. The members of F6 are part of the EUROfusion consortium, which works in the fields of fusion-related research, following the current plan to confirm the operational principle of nuclear fusion. Currently, the main research is triggered by the ITER project, which is being built in Cadarache in France. The accelerated phases of the construction of the rector and the associated subassemblies are being finalised after a standstill. It will be the biggest fusion reactor with the main purpose to demonstrate the feasibility of the concept of tokamak with the gain of the input energy by a factor of 10. Its last version will be created before the first fusion power plant will be built. Our current research program focuses on the interactions of hydrogen isotopes with the structural materials used for fusion purposes. When it comes to physical nuclear reactions in fission processes, care must be taken when handling unused fuel and reaction products. When exploiting fusion energy, the amount of radioactive materials is very small but not negligible. The retention of radioactive tritium in the materials is difficult to control because it easily penetrates the reactor's metal walls from where it could leak into the environment through the cooling system.

Tritium retention can be predicted fairly accurately based on the research and experiments that can be performed with hydrogen and deuterium, as they are all chemically similar. Much of the research in the group was the evaluation of retained deuterium in various samples received from several labs within the EUROfusion consortium. Our main technique is thermal desorption spectroscopy (TDS) with an *in situ* calibrated quadrupole mass spectrometer. For improving its reliability we made an innovative study of the interference effect.

The quantification of the data recorded by quadrupole mass spectrometers requires a careful analysis of all contributions influencing the proportionality of the ion current conversion to the gas flow rate. We proposed a novel calibration protocol with a subsequent mathematical analysis that increases the quantification accuracy when one of the two gases in a mixture substantially influences the other gas's detection sensitivity. The phenomenon known as the interference effect depends on the magnitude of the gas flow rates and their ratio. Deuterium and argon were selected to demonstrate the efficiency of the proposed schedule for reducing the error below ˜ 10%. The error of deuterium evaluation at particular flow rate ratios would be ∼2.5 times higher when ignoring the argon impact.

The divertor is likely to operate on a different basis in the next generation of reactors than in ITER. Among the possible concepts, an attractive divertor has been used for many years. The liquid metal trapped in the tungsten porous support structure continuously dissipates the heat flow into the cooling system so that the surface itself is not damaged even in the event of plasma instability. In the research, we studied tin, an extremely interesting candidate for the described concept due to its low melting point of around 220 ° C. When exposing tin to atomic deuterium, we found that most deuterium was bound to tin oxide. Tin itself is completely inert to deuterium, although we observed an extremely low concentration, ∼1 ppb D/Sn.

Plasma-enabled design of hybrid carbon nanostructures for energy-related applications. Carbon nanostructures have significant potential in energy storage and conversion applications, considering their easy functionalization and tailoring features. The members of F6 devoted significant efforts to designing hybrid graphene and carbon-based nanostructures for energy-related applications in the last year. We established a fast and facile, two-step method for fabricating an advanced hybrid electrode consisting of trinickel disulphide (Ni_3S_2) formed on metallic Ni nanoparticles supported by a vertical carbon nanotube (VCN) backbone in the form of Ni_3S_2/Ni@VCN. This was achieved with the plasma deposition of VCNs, followed by low-temperature annealing in the presence of H_2S. The active material had direct contact with the current collector due to direct plasma deposition, enabling a good electrical contact. Also, the resulted active material possesses a hierarchical morphology with a broccoli structure (Figure 6). The designed Ni_3S_2/Ni@VCN electrode was tested as the anode material for lithium-ion batteries. The electrode featured outstanding lithium-storage capabilities with a high reversible capacity (1113 mAh g^{-1} after 100 cycles at 100 mA g^{-1}), excellent long-term cycling stability (770 mAh g^{-1} after 500 cycles at 200 mA g^{-1}) and good rate capability. The obtained performance is one of the best Li-ion storage capabilities of the Ni_3S_2-type anode materials. The electrode fabrication technique employed is one of the fastest methods for fabricating high-performance Ni_3S_2-based binder-free electrodes. Also, the unique "broccoli-like" structure of polycrystalline Ni_3S_2 capped on a

conductive VCN backbone helps the interface storage process and boosts the lithium storage performance, providing a path toward the next-generation energy storage devices of the future.

The collaboration with the researchers from Instituto Superior Técnico, Lisbon, Portugal, enabled also the development of a ground-breaking plasma-enabled green approach for engineering graphene-related structures to design energy storage materials for sustainable energy storage systems. The research demonstrates one of the fastest methods for synthesizing nitrogen-doped graphene and incorporating metal oxide (sulphide) nanoparticles into graphene layers, simultaneously using a microwave plasma system. Hybrid N-graphene (nitrogen-doped graphene) metal-based nanostructures were produced at a rate of ∼ *19 mg/min, one of the fastest production rates in an* environment-friendly way. In addition, nano-sized (∼10–30 nm) MnO$_x$ *particles and oxidized metal* sulphide particles were intercalated between the N-graphene sheets at atmospheric conditions by spraying the precursors in plasma. The hybrid nanostructures exhibited promising energy storage capabilities and stability when acting as a supercapacitor electrode. The chemically engineered process is expected to significantly impact the design of advanced electrode materials for sustainable energy storage systems.

Figure 8: Schematic of the charge pathways in the plasma-designed broccoli-like Ni_3S_2/Ni@VCN electrode material; structural defects of the Ni_3S_2/Ni@VCN material are in the inset.

The collaboration with the researchers from GREMI (Groupe de Recherches sur l'Energétique des Milieux Ionisés), Orléans, France, continued, including the research of designing carbon nitride nanostructures with high thermal stabilities. The team established a green approach for designing hydrogenated nitrogen-rich carbon nitride nanoparticles using a low-pressure, low-power, plasma-deposition technique from a methane/nitrogen gas mixture. Advanced near-edge X-ray absorption fine-structure spectroscopy (NEXAFS, *in-situ*) was used to evaluate the thermal stabilities of the designed nanostructures at high temperatures. Thermal studies revealed an excellent stability of the material and nitrogen-rich characteristics (N/C ratio of 0.5–0.2 ± 0.01). The obtained results indicate a transformation of sp^3-rich as-deposited carbon nitride into an sp^2-carbon phase with more graphitic features upon thermal annealing, and the designed material exhibits stability even at a temperature of above 1100 K. Additionally, the team showed that these thermally stable structures transform a hydrophilic surface into a hydrophobic one upon annealing and revealed that this type of surface can be appropriate for hydrophobic surface coatings, used in harsh conditions.

Figure 9: Schematic representation of a plasma system for the production of metal derivatives intercalated between N-graphene sheets

The development of hybrid carbon nanostructures is important for high performing device applications and it is one of our major tasks within the H2020 FET-Open project PEGASUS. All the developed methods and achieved/measured performances were presented in high-impact journals.

Some outstanding publications in the past year

1. Neelakandan Marath Santhosh, Kush K. Updhyay, Petra Stražar, Gregor Filipič, Janez Zavašnik, Andre Mão de Ferro, Rui Pedro Silva, Elena Tatarova, Maria de Fátima Montemor, Uroš Cvelbar, Advanced carbon-nickel sulfide hybrid nanostructures: extending the limits of battery-type electrodes for redox-based supercapacitor applications, *ACS Applied Materials & Interfaces*, 2021, vol. 13, iss. 7, 20559–20572, illustr., ISSN 1944-8244, DOI: 10.1021/acsami.1c03053.

2. Ivana Sremački, Špela Kos, Maša Bošnjak, Andrea Jurov, Gregor Serša, Martina Modic, Christophe Leys, Uroš Cvelbar, Anton Nikiforov, Plasma damage control: from biomolecules to cells and skin, *ACS Applied Materials & Interfaces*, 2021, vol. 13, no. 39, 46303–46316, ISSN 1944-8244, DOI: 10.1021/acsami.1c12232.

3. Constantinos M. Damaskinos, Janez Zavašnik, Petar Djinović, Angelos M. Efstathiou, Dry reforming of methane over Ni/Ce0.8Ti0.2O2–δNi/Ce0.8Ti0.2O2–δ: the effect of Ni particle size on the carbon pathways studied by transient and isotopic techniques, *Applied Catalysis B, Environmental*, [Print ed.], 2021, vol. 296, 1–20, ISSN 0926-3373, DOI: 10.1016/j.apcatb.2021.120321.

4. Anand Mohan Shrivastav, Uroš Cvelbar, Ibrahim Abdulhalim, A comprehensive review on plasmonic-based biosensors used in viral diagnostics, *Communications Biology*, 2021, vol. 4, 70-1-70-12, ISSN 2399-3642, DOI: 10.1038/s42003-020-01615-8.

5. Neelakandan Marath Santhosh, Nitheesha Shaji, Petra Stražar, Gregor Filipič, Janez Zavašnik, Chang Won Ho, Nurugan Nanthagopal, Chang Woo Lee, Uroš Cvelbar, Advancing Li-ion storage performance with
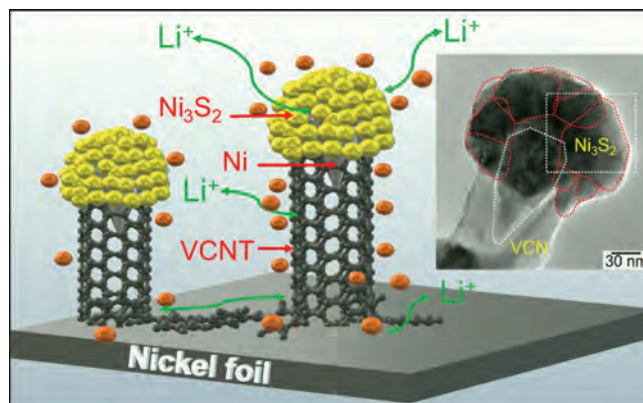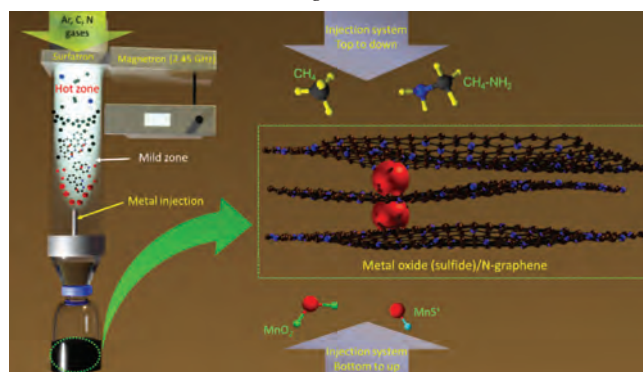
hybrid vertical carbon/Ni3S2Ni3S2-based electrodes, *Journal of Energy Chemistry*, 2022, vol. 67, 8–18, ISSN 2095-4956, DOI: 10.1016/j.jechem.2021.09.034.

6. Nataša Hojnik, Martina Modic, James L. Walsh, Dušan Žigon, Uroš Javornik, Janez Plavec, Bojana Žegura, Metka Filipič, Uroš Cvelbar, Unravelling the pathways of air plasma induced aflatoxin B1B1 degradation and detoxification, *Journal of Hazardous Materials*, [Print ed.], 2021, vol. 403, 1–29, illustr., ISSN 0304-3894, https://www.sciencedirect.com/science/article/pii/S030438942031579X, DOI: 10.1016/j.jhazmat.2020.123593.

7. Vincenc Nemanič, Janez Zavašnik, Vasyl Shvalya, Marko Žumer, Hydrogen permeability of non-stoichiometric tungsten oxides, *Journal of Nuclear Materials*, [Print ed.], 2021, vol. 548, 152860-1-152860-8, illustr., ISSN 0022-3115, DOI: 10.1016/j.jnucmat.2021.152860.

8. Sanghoo Park, Wonho Choe, Hyungyu Lee, Joo Young Park, Jinwoo Kim, Se Youn Moon, Uroš Cvelbar, Stabilization of liquid instabilities with ionized gas jets, Nature, [Print ed.], 2021, vol. 592, 49–53, ISSN 0028-0836, DOI: 10.1038/s41586-021-03359-9.

9. Ines Hamouda, Cédric Labay, Uroš Cvelbar, Maria-Pau Ginebra, Cristina Canal, Selectivity of direct plasma treatment and plasma-conditioned media in bone cancer cell lines, *Scientific Reports*, 2021, vol. 11, 17521-1-17521-12, ISSN 2045-2322, DOI: 10.1038/s41598-021-96857-9.

10. Neelakandan Marath Santhosh, Vasyl Shvalya, Martina Modic, Nataša Hojnik, Janez Zavašnik, Jaka Olenik, Martin Košiček, Gregor Filipič, Ibrahim Abdulhalim, Uroš Cvelbar, Label-free mycotoxin raman identification by high-performing plasmonic vertical carbon nanostructures, *Small*, 2021, vol. 17, iss. 49, 2103677-1-2103677-11, ilustr., ISSN 1613-6829, DOI: 10.1002/smll.202103677.

Awards and Appointments

1. Uroš Cvelbar, Martina Modic, et al. Golden Award for Innovation of the Chamber of Commerce of Dolenjska and Bela Krajina 2021.

2. Nataša Hojnik, Award of Slovenian Research Agency – Excellent in Science 2021, Unravelling the pathways of air plasma induced aflatoxin B1 degradation and detoxification.

Patent granted

1. Gregor Filipič, Kristina Eleršič, Darij Kreuh, Janez Kovač, Uroš Cvelbar, Miran Mozetič, A method of colouring titanium and titanium alloys, GB2530805 (B), Intellectual Property Office, 24. 11. 2021.

INTERNATIONAL PROJECTS

1. Max Planck Partner Group
   Asst. Prof. Janez Zavašnik
   Max-Planck-Institut Für Eisenforschung GmbH
2. COST CA18113; Understanding and Exploiting the Impact of Low pH on Microorganisms
   Dr. Martina Modic
   Cost Association Aisbl
3. COST CA18116; Aniridia: Networking to Address an Unmet Medical, Scientific and Societal Challenge
   Prof. Uroš Cvelbar
   Cost Association Aisbl
4. COST CA19110; Plasma Applications for Smart and Sustainable in Agriculture
   Dr. Martina Modic
   Cost Association Aisbl
5. NATO: NOOSE - Nanomaterials for Explosive Traces Detection with SERS
   Prof. Uroš Cvelbar
   Nato - North Atlantic Treaty Organisation
6. COST CA20120 - Therapeutical Applications of Cold Plasma
   Dr. Martina Modic
   Cost Association Aisbl
7. COST CA20129 - Multiscale irradiation and chemistry driven processes and related technologies
   Prof. Uroš Cvelbar
   Cost Association Aisbl
8. H2020 - PEGASUS; Plasma Enabled and Graphene Allowed Synthesis of Unique nano Structures
   Prof. Uroš Cvelbar
   European Commission
9. H2020 - EUROfusion; Plasma Facing Components-1-IPH-FU, EUROfusion

Dr. Vincenc Nemanič
European Commission
10. H2020 - EUROfusion; WPPFC-PEX-FU, WPPFC-PEX-FU, EUROfusion
    Dr. Vincenc Nemanič
    European Commission
11. Investigation of Helium Retention in Plasma Facing Materials Using Advanced Analytical Methods
    Asst. Prof. Janez Zavašnik
    Slovenian Research Agency
12. Oxidative Stress Responses of Microbial Biofilms Exposed to Cold Atmospheric Pressure Plasma Generated Reactive Species
    Dr. Martina Modic
    Slovenian Research Agency
13. Designing Catalytic Activity of Nanomaterials with Plasma
    Prof. Uroš Cvelbar
    Slovenian Research Agency
14. Beyond Graphene - The New Materials based on 2D and 3D Graphene
    Prof. Uroš Cvelbar
    Slovenian Research Agency
15. Exploration of Metal/Metal-Oxide Sensor Capabilities
    Dr. Gregor Filipič
    Slovenian Research Agency
16. Designing Plasmonicity of Carbon-Based Nanomaterials
    Prof. Uroš Cvelbar
    Slovenian Research Agency
17. HE - EUROfusion; WP07: ENR-DeHydroc-1,2,3_HE-FU
    Asst. Prof. Janez Zavašnik
    European Commission
18. HE - EUROfusion; WP18: MAT_HE-FU, IREMEV-MAT-1_HE-FU, IREMEV-MAT-2_HE-FU, IREMEV-MAT-3_HE-FU

Asst. Prof. Janez Zavašnik
European Commission
19. HE - EUROfusion; WP05: PWIE-1,2,3_HE-FU
Dr. Vincenc Nemanič
European Commission

RESEARCH PROGRAMMES

1. Vacuum technique and materials for electronics
   Dr. Vincenc Nemanič
2. Thin film structures and plasma surface engineering
   Prof. Uroš Cvelbar

R & D GRANTS AND CONTRACTS

1. Plasma In-situ reactions and single crystal Transitions
   Prof. Uroš Cvelbar
2. Hybrid and Reengineered Nanocatalysts for New Purification Routes
   Prof. Uroš Cvelbar
3. Plasma decontamination of mycotoxins and inactivation of fungi in food industry
   Dr. Martina Modic

4. Controlling plasma-bio interactions for global food security
   James Leon Walsh
5. Detection of defects and hydrogen by ion beam analysis in channelling mode for fusion
   Asst. Prof. Janez Zavašnik

VISITORS FROM ABROAD

1. Prof. Danijela Vujošević, Institute of Public Health, Podgorica, Montenegro, 17–20 September 2021

2. Prof. Oleg Baranov, University of Kharkiv, Kharkiv, Ukraine, 8–20 November 2021

STAFF

Researchers
1. Prof. Uroš Cvelbar, Head
2. Dr. Gregor Filipič
3. Dr. Martina Modic
4. Dr. Vincenc Nemanič
5. Dr. Vasyl Shvalya
6. Dr. James Leon Walsh
7. Asst. Prof. Janez Zavašnik

Postdoctoral associates
8. Dr. Nataša Hojnik

9. Dr. Neelakandan Marath Santhosh

Postgraduates
10. Martin Košiček, B. Sc.
11. Marko Žumer, B. Sc.

Technical officers
12. Jaka Olenik, B. Sc.
13. Damjan Vengust, B. Sc.

Technical and administrative staff
14. Urška Kisovec, B. Sc.

BIBLIOGRAPHY

ORIGINAL ARTICLE

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5. Andrea Jurov, Špela Kos, Nataša Hojnik, Ivana Sremački, Anton Nikiforov, Christophe Leys, Gregor Serša, Uroš Cvelbar, "Analysing mouse skin cell behaviour under a non-thermal kHz plasma jet", *Applied sciences*, 2021, **11**, 3, 1266.

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THESES AND MENTORING

1. Andrea Jurov, *Optical emission spectroscopy as a tool for monitoring cold atmospheric pressure plasma processes:* doctoral dissertation, Ljubljana, 2021 (mentor Uroš Cvelbar; co-mentor Nataša Hojnik).
2. Neelakandan Marath Santhosh, *Plasma-enabled design of hybrid carbon nanostructures for energy storage applications:* doctoral dissertation, Ljubljana, 2021 (mentor Uroš Cvelbar; co-mentor Gregor Filipič).

DEPARTMENT FOR COMPLEX MATTER

The research within the Department of Complex Matter encompasses a variety of research fields, ranging from fundamental investigations of elementary excitations in quantum materials, nonequilibrium quantum matter, self-organizing behaviour adaptive functionality in complex systems and soft matter as well as nano-biosystems, biomolecules and various nanomaterials. The department's experimental activities are strongly complemented by theory on different levels and supported by diverse materials synthesis. Our research into ultrafast non-equilibrium transitions, investigations of new emergent hidden orders and ferromagnetic liquids are of significant interest worldwide.

The experimental methods used at the department are suitably diverse, from different femtosecond laser spectroscopies from THz to XUV, a variety of optical techniques, ultrafast transport and superconducting devices studies as well as synthetic chemistry and thin-film deposition methods such as MBE, ALD and EBE, laser biomedical studies, femtosecond STM and magnetometry.

Head:

Prof. Dragan D. Mihailović

European Research Council
Established by the European Commission

The experimental research within the department is strongly supported by theory, ranging from analytical approaches to modelling with Monte-Carlo simulations. **Quantum annealing on a D-wave quantum computer** has become a useful technique for modelling non-equilibrium phenomena.

A number of spin-out research projects have recently gained importance, most recently ultrafast, low-energy cryo-memory devices based on our studies of ultrafast electronic transitions.

The research achievements are thus quite diverse, and we are able to report on important discoveries in a number of areas.

Quantum billiards

Forcing systems through fast non-equilibrium phase transitions offers the opportunity to study new states of quantum matter that self-assemble in their wake. In 2021 we reported a study of the quantum-interference effects of correlated electrons confined in monolayer quantum nanostructures, created by a femtosecond, laser-induced quench through a first-order polytype structural transition in a layered transition-metal dichalcogenide material. Scanning tunnelling microscopy of the electrons confined within equilateral triangles, whose dimensions are a few crystal unit cells on the side, reveals that the trajectories are strongly modified from free-electron states both by electronic correlations and confinement. A comparison of experiments with theoretical predictions of strongly correlated electron behaviour reveals that the confining geometry destabilizes the Wigner/Mott crystal ground state, resulting in mixed itinerant and correlation-localized states intertwined on a length scale of 1 nm. The work opens the path towards understanding the quantum transport of electrons confined in atomic-scale monolayer structures based on correlated-electron materials. The paper was published in **Nature Communications, (2021) 12, 3793 (2021).** A video presentation of the work was recorded by the Slovenian media (STA) and is available on YouTube channel (https://youtu.be/yqorfqrGrMk)

A time-domain phase diagram of 1T-TaS$_2$

Metastable self-organized electronic states in quantum materials are of fundamental importance, displaying emergent dynamical properties that can be used in new generations of sensors and memory devices. Such states are typically formed through phase transitions under non-equilibrium conditions and the final state is reached through processes that span a large range of timescales. Conventionally, phase diagrams of materials are thought of as static, without temporal evolution. However, many functional properties of materials arise because of complex temporal changes in the material occurring on different timescales. Hitherto, such properties were not considered
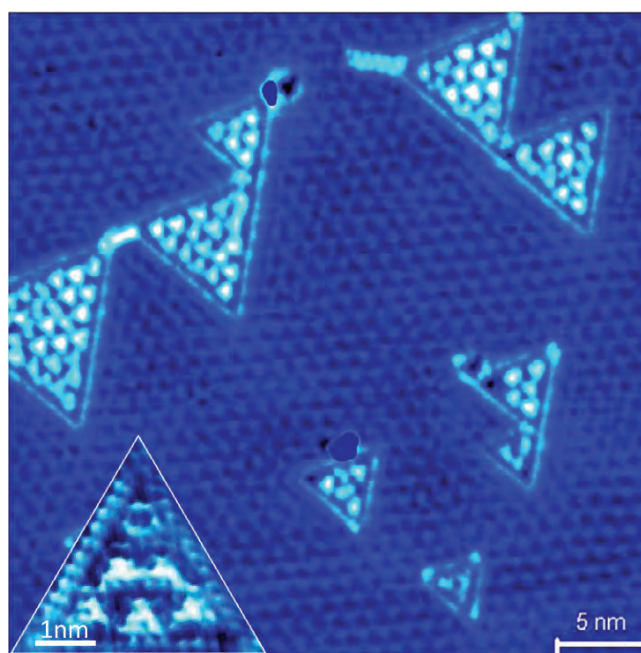

Figure 1: Quantum billiards inside equilateral triangles formed in a 1T/1H TaS$_2$ heterostructure/nanostructure. The electron-density maps show localized, itinerant and edge states.

within the context of a temporally evolving phase diagram, even though, under non-equilibrium conditions, different phases typically evolve on different timescales. Here, by using time-resolved optical techniques and femtosecond-pulse-excited scanning tunnelling microscopy (STM), we track the evolution of the metastable states in a material that has been of wide recent interest, the quasi-two-dimensional dichalcogenide 1T-TaS$_2$. We map out its temporal phase diagram using the photon density and temperature as control parameters on timescales ranging from 10^{-12} to 10^3 s. The introduction of a time-domain axis in the phase diagram enables us to follow the evolution of metastable emergent states created by different phase-transition mechanisms on different timescales, thus enabling a comparison with theoretical predictions of the phase diagram, and opening a way to understanding the complex ordering processes in metastable materials. The work was published in **Nature Communications, 12, 2323 (2021)**.

Charge Configuration Memory devices

In 2021 major progress was made in the fabrication, testing and modelling of charge-configuration memory (CCM) devices. CCM devices are an original invention based on the discovery of a hidden charge-ordered state in the transition-metal dichalcogenide published in **Science** (2014), with follow up publications in **Nature Communications** (2016), **npjQM** (2018), **Nat. Comm** (2021), **Nature Materials** (2019), **Science Advances** (2015) amongst others.

CCM device operation is based on the controllable reconfiguration of electronic domains in a charge-density wave material. Since the dominant effect involves the manipulation of electrons rather than atoms, the devices can display a sub-picosecond switching speed and an ultralow, few-femtojoule switching energy. The mechanisms involved in switching between the domain states of different electrical resistances are highly non-trivial and involve trapping non-equilibrium charges within topologically protected domain states. In a letter, prepared in response to an invitation by the Editors of Applied Physics Letters, we discuss the underlying physics that is deemed essential for the operation of CCM devices, focusing on the unusual asymmetry between non-thermal "write" processes and thermal "erase" processes from the point of view of the mechanism in relation to the thermal dynamics. The results also appeared on the cover page of **Appl. Phys. Lett. 119, 013106 (2021)**.

Figure 2: Cover of Applied Physics Letters

In four further publications currently under review, different aspects of the device are discussed. The first presents Ultra-Efficient Resistance Switching between Charge Ordered Phases in 1T-TaS$_2$ with a Single Picosecond Electrical Pulse (arXiv:2202.13831). In the second publication we investigate the energy efficiency scaling of such CCM devices as a function of device size and data write time τ_w as well as other parameters, which have a bearing on efficient device operation. We find that the switching energy efficiency scales approximately linearly with both quantities over multiple decades, departing from linearity only when τ_w approaches the ~0.5 ps intrinsic switching limit. Compared to the current state-of-the-art memory devices, CCM devices are found to be much faster and significantly more energy efficient, demonstrated here with two-terminal switching using 2.2 fJ, 16 ps electrical pulses. (arXiv:2103.04622). The third publication, using multi-probe scanning tunnelling microscopy (STM), we investigate microscopically how non-trivial topological defects in the electronic domain structure reconfigure in response to an applied current within an operational device. The defects, which are topologically equivalent to conventional crystal dislocations, appear robust at small currents. At higher currents, they show pairwise annihilation that directly correlates with a change of the sample's electrical resistance. The conspicuous absence of CDW sliding under a lateral field, and the clear distinction between thermally activated domain relaxation processes and T-independent resistivity implies the presence of an unconventional 2-component charge-transport mechanism that can be modulated by the manipulation of the domain structure. In a fourth publication (arXiv:2203.14586) we present an implementation of non-volatile CCM in a cryo-computing environment by combining it in parallel with a pulse-triggered superconducting nanowire cryotron (nTron). The combined device is modelled in terms of the dynamical response of the SC order parameter in a current-controlled nanowire with a CCM shunt. Analysis of time dynamics and current-voltage characteristics based on measured device parameters show that single flux quantum (SFQ)-level pulses can drive a non-volatile CCM on the picosecond timescale, while allowing the nTron to operate in non-latching mode. The inherent high energy efficiency and ultra-high speed makes this hybrid device an ideal memory for use in cryo-computing and quantum computing peripheral devices.

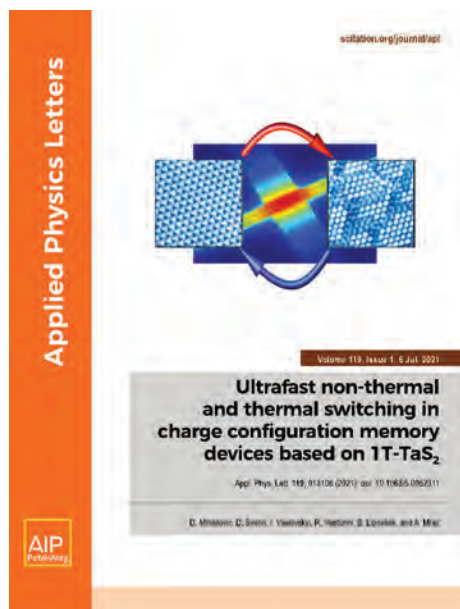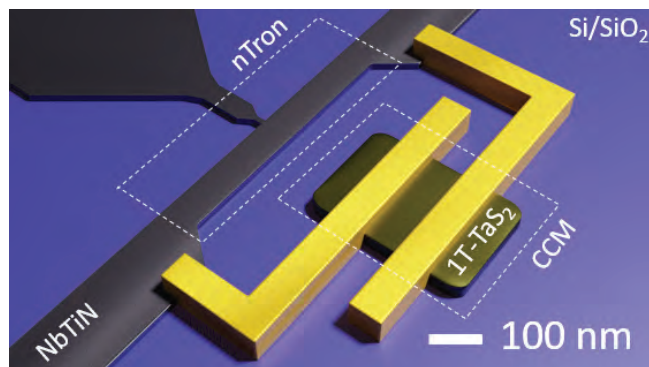*Figure 3: 3D model of the combined device. nTron is made from NbTiN thin film (grey), CCM is 1T-TaS$_2$ crystal (dark yellow-green) and golden electrodes connect them together in parallel (bright yellow). Entire circuit is on a Si/SiO$_2$ substrate (violet).*

Ultrafast studies of non-equilibrium quantum matter

We continued the study of intense femtosecond optical pulse irradiation effects in $CuIr_2S_4$ by means of the all-optical ultrafast multi-pulse time-resolved spectroscopy. The data suggest that the photoinduced-transition dynamics to the High-T metallic phase is governed by first-order-transition nucleation kinetics that prevents the complete ultrafast structural transition even when the absorbed energy significantly exceeds the equilibrium enthalpy difference to the high-T metallic phase. In contrast, the dynamically decoupled electronic order is transiently suppressed on a sub-picosecond timescale rather independently due to a photo-induced Mott transition as reported in **New Journal of Physics, 23, 053023 (2021)**.

The effect of disorder in high-T_c superconductors was investigated from the viewpoint of photo-induced quasiparticle (QP) dynamics, obtained by means of the time-resolved pump-probe spectroscopy. We performed measurements in an optimally doped $Bi_{2+x}Sr_{2-x}CaCu_2O_{8+\delta}$ (Bi2212) with an out-of-plane disorder induced by Bi-Sr substitution (x), which is present in standard Bi2212 but is not usually controlled. Based on the systematic change of the disorder with controlled x, we identified the changes in the dynamics of QP relaxation and gap formation in superconducting (SC) and pseudo-gap (PG) states. The onset temperature T^* of the PG response increases with an increase in x, which is more significant than the slight decrease in T_c. These properties are equivalently reflected in the destruction fluences of the SC and PG states. Bi-Sr substitution also accelerates the relaxation times for SC and PG QPs, which can be due to the increased phonon scattering probability caused by the disorder. In contrast, the SC gap recovery observed in the strongly excited condition shows an identical fluence dependence for various x, implying that the disorder does not significantly contribute to the coherent gap formation as published in **Phys. Rev. B 104, 094507 (2021)**.

We investigated the quench and real-time formation of the Mott state and photo-excited carrier relaxation dynamics in the Mott insulator κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl (κ-Cl) and the superconductor κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br (κ-Br) using three-pulse femtosecond optical spectroscopy, where BEDT-TTF is bis(ethylenedithio)tetrathiafulvalene. In both salts

Figure 4: A schematic illustration of the time evolution of electronic states after the intense femtosecond laser pulse irradiation in strongly correlated organic salts κ-Cl and κ-Br.

we find that transient reflectivity amplitude gradually recovers with time after strong near-infrared pulse quench, but its relaxation time is nearly constant throughout. This indicates that in κ-Cl the energy gap for charge excitations is filled rather than closed by photo-induced carriers of only ~0.5% per dimer. The Mott state is re-formed on a few-picosecond timescale with disappearance of the in-gap photo-doping-induced states near the Fermi energy. In κ-Br, a behaviour similar to that in κ-Cl is observed and attributed to the disorder-induced phase-separated Mott insulating regions as published in **Phys. Rev. B 104, 115152 (2021)**.

Theoretical studies on the nanoscale

Metastable self-organized electronic states in quantum materials are of fundamental importance, displaying emergent dynamical properties that can be used in new generations of sensors and memory devices. Such states are typically formed through phase transitions under non-equilibrium conditions and the final state is reached through processes that span a large range of timescales. By using time-resolved optical techniques and femtosecond-pulse-excited scanning tunnelling microscopy, the evolution of the metastable states in a material that has been of wide recent interest, the quasi-two-dimensional dichalcogenide 1T-TaS$_2$ was observed. To describe the experimental observations, we use state-of-the-art Monte Carlo simulations of a charge lattice gas of polarons in order to predict the experimental phase diagram. Our generic model predicts the structure of the experimental phase diagram almost entirely, except for the 1/12 phase, which is not found experimentally. This finding elucidates the importance of other mechanisms in the formation of the equilibrium phases other than only polaronic correlations. The results of this theory were published in **Nature communications, 12, 3793 (2021)**.

Forcing systems through fast non-equilibrium phase transitions offers the opportunity to study new states of quantum matter that self-assemble in their wake. The quantum-interference effects of correlated electrons confined in monolayer quantum nanostructures, created by femtosecond laser-induced quench through a first-order polytype structural transition in a layered transition-metal dichalcogenide material was studied experimentally. The scanning tunnelling microscopy of the electrons confined within equilateral triangles, whose dimensions are a few crystal unit cells on the side, reveals that the trajectories are strongly modified from free-electron states both by electronic correlations and confinement. A comparison of experiments with theoretical predictions of strongly correlated electron behaviour reveals that the confining geometry destabilizes the Wigner/Mott crystal ground state, resulting in mixed itinerant and correlation-localized states intertwined on a length scale of 1 nm. Our Monte Carlo
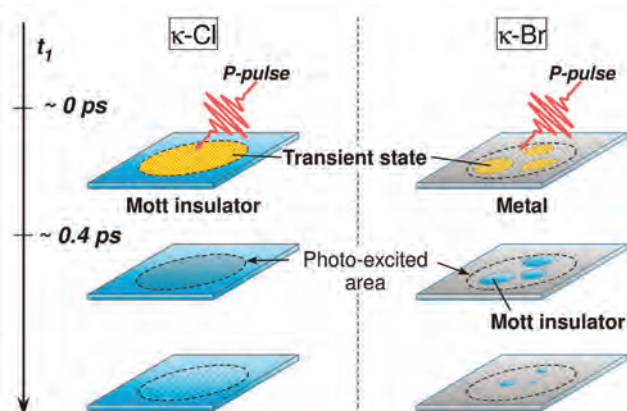
simulations show that polaronic configurations deform significantly in small tringles, whereas the deformation is localized more towards the edge, the larger the triangle is. The natural quantum extension of the same model reveals that electrons delocalize significantly more in the cases where frustration due to confinement is larger and already apparent in classical simulations. Theoretical simulations therefore conclude that geometrical frustration due to the confinement of polarons is the main driver of the experimentally observed quantum-interference patterns. The work opens the path towards understanding the quantum transport of electrons confined in atomic-scale monolayer structures based on correlated-electron materials. The results of this theory were published in **Nature communications**, 12, 3793 (2021).

Nanomaterials

Transition-metal carbides and nitrides with large surface areas are in general attractive for various catalytic reactions. We explored the possibility to produce molybdenum-based nitride and carbide heterostructures from two nanowires precursors (MoSI and MoOxideAniline nanowires) by heating in NH_3 and ethane/hydrogen/argon gas mixtures. This novel synthetic route presents a technologically viable, easily scalable and controllable method for producing molybdenum carbide/nitride nanowires composed of around 10-nm grains. The catalysts composed of pure nitride phases demonstrate higher CO chemisorption for samples prepared from MoOxideAniline NWs than MoSI NWs with a value of $4.2 \, \mu mol \, g^{-1}$. All the samples show catalytic activity for CO_2 reduction and excellent selectivity to CO production. Despite the small variation in surface composition and structural rearrangement after the repeated catalytic process the material exhibits long-term stability at a moderate conversion rate. A high selectivity towards CO was further investigated. By repeating the experiments with varying CO_2-to-H_2 ratios, the Mo_2C/Mo_2N nanowires showed a higher CO_2 conversion compared to Mo_2C. The stability of the Mo_2C/Mo_2N catalyst tested at 300 °C showed high stability over a long period of time (>24 h) and had a high selectivity towards CO preserved at around 99%.The comparison of catalyst characterisation before and after the RWGS reaction shows that there is no major difference in the physical and chemical characteristics of the materials further validate the use of the present catalysts. This work was published in journal **Renewable Energy**.

Figure 5: The global carbon footprint can be mitigated by utilizing the renewable nature of CO2, where it could be captured, stored, and used for the production of various fuels through carbon capture and utilization technology. A highly promising path is a direct Fischer-Tropsch type process in one reactor with a reverse water gas shift reaction (RWGS) using carbon dioxide in combination with hydrogen as a feed mixture. The RWGS reaction is an equilibrium reaction limited to high temperatures due to the endothermic nature of the reaction $CO_2 + H_2 \leftrightarrow CO + H_2O$. CO2 is a highly stable and rather inert molecule, so it is of great importance to developing stable, highly active, and selective catalysts in both reductions.

We have contributed measurements of photoluminescence exhibited by TiO_2 nanotubes immobilized on titanium foils and supported additional analyses looking into relationships between their synthesis conditions and composition, structure, and UV photocatalytic properties. (Collaboration with Department for Nanostructured Materials and Department of Surface Engineering, IJS, and National Institute of Chemistry) as published in **ACS Omega 6, 23233, (2021)**.

Soft Matter

We investigated the mechanisms of G-quadruplex formation in the DNA sequences $(G_4C_2)_n$ associated with neurological disorders ALS and FDT. We found that the sequences with n=1, 2, and 4 exhibit very different folding topologies and consequently possess different macromolecular association properties (**International Journal of Molecular Sciences 22, 4532 (2021)**. We continued with investigations of Langmuir films of DNA nucleoside derivatives at the air-water interface and Langmuir-Blodgett films on solid substrates. The emphasis was on the photo-isomerization process in azo-functionalized guanosine derivatives. We found that such derivatives are promising candidates for the fabrication of photo-active 2D materials that can provide all the beneficial functionalities of DNA-based compounds (**ACS Omega 6, 15421 (2021)**). The Langmuir-Blodgett method was also used to fabricate protective monolayer coatings against the high-temperature corrosion of concentrating solar-power absorber surfaces (**Solar Energy Materials and Solar Cells 223, 110984 (2021)**.

In cooperation with researchers from Nankai University in China we continued to investigate tuneable optical diffraction structures based on liquid
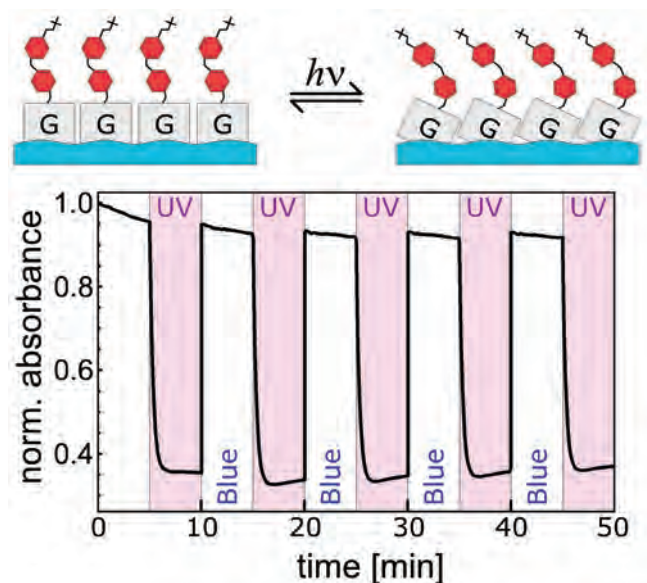

Figure 6: Temporal modifications of normalized absorbance at 330 nm detected in chloroform solutions of photosensitive guanosine derivative during alternating irradiations with blue and UV light. Intervals of UV irradiation are shaded in violet.
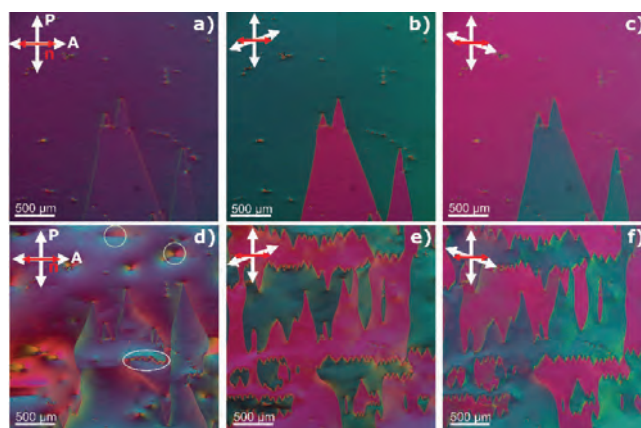
crystals that are introduced into laser-written polymeric scaffolds (our patent WO2015139353 (A1). A theoretical work on electrically tuneable optical diffraction gratings fabricated by introducing a conventional nematic liquid crystal mixture into such scaffolds was reported in **Polymers 13**, 2292 (2021). We also investigated light propagation in cholesteric liquid crystals introduced into the periodic assembly of polymeric ribbons with planar surface anchoring (**Physical Review E 104**, 064702 (2021)).

In collaboration with researchers from the East Bavarian Technical High School (OTH) in Regensburg and the Faculty of Mechanical Engineering at University of Ljubljana we investigated various aspects of magnetically regulable surface properties of magneto-active elastomers (MAEs). MAEs are composite materials comprised from magnetic microparticles embedded in a soft elastomer matrix. We showed that characteristics of liquid drop splashing on surface of MAEs can be tuned with a magnetic field (**Advanced Materials Interfaces 8**, 1 (2021). We demonstrated that laser micromachining of MAEs can be used to fabricate surface micropatterns of various sizes and shapes (**Advanced Materials Technologies 2021**, 2101045). We also demonstrated that reconfigurable micropatterns can be imprinted into MAE surface based on the magnetic field-induced shape memory effect (**Polymers 13**, 4422 (2021).

We continued the investigations of ferroelectric nematic liquid crystals. We studied the molecular origin of polar ordering by comparing, both experimentally and by means of molecular dynamic simulations, two materials with similar chemical structure and demonstrate that a subtle molecular change enables denser packing when they exhibit polar order. Such a reduction of the excluded volume lies in the origin of the polar nematic phase. This study also shows how MD simulations can be used for molecular design, by predicting and identifying candidate materials for the polar or its precursor nematic phases (**Nat Commun 12**, 4962 (2021)). **We** also examined the formation and structure of large polar nematic domains of the ferroelectric nematic material RM734 in planar liquid-crystal cells with different aligning agents and specifications. We observed that confining surfaces have a strong influence over the formation of different types of domains, resulting in various twisted structures of the nematic director. For those cells predominantly showing mm-scale domains, we investigated the optical and second harmonic generation switching behaviour under applications of electric fields with a special focus on in-plane fields perpendicular to the confinement media rubbing direction. To characterize the underlying structure, the polar optical switching behaviour was reproduced using a simplified model together with Berreman calculations (**Liquid Crystals 48**, 2055 (2021)).

Figure 7: Polarized microscope images of domain division/creation by application of out of plane fields in a 5.4-micrometre-thick layer of ferro-electric nematic liquid crystal. Before application of field between crossed polarisers (a), and with analyser uncrossed (b,c). (d) Texture observed during the application of 1 Hz square-wave field of Vp = 1.5 V. (e,f) Final state of the sample after the field is switched off. (Reproduced from Liquid Crystals 48, 2055 (2021), published under CC BY-NC-ND 4.0).

We studied ferromagnetic ordering in suspensions of magnetic barium-hexaferrite nanoplatelets in isotropic solvents, which above certain threshold concentrations of the nanoplatelets exhibit a transition to the ferromagnetic nematic phase. The key interactions between the platelets are long-range dipolar magnetic and screened anisotropic electrostatic. We tuned the isotropic-nematic phase transition in 1-butanol ferrofluids of BHF NPLs by affecting the interactions in the ferrofluids. We observed that the threshold concentration (typically around 5%(v/v)) decreased by 0.6 % (v/v) with a larger mean diameter of the platelets, up to 0.6 % (v/v) with increased ionic strength of the ferrofluid, and for about 2 % (v/v) with higher saturation magnetization of the platelets. We showed that by tuning the parameters affecting the ferrofluid's interplatelet interactions, we can alter the threshold concentration for the liquid magnet formation. The results elucidate the importance of a delicate balance between the repulsive screened electrostatic and attractive dipolar magnetic interactions for the liquid magnet formation (**Journal of Molecular Liquids 118038 (2021)**). We also contributed to the development of barium-hexaferrite/gold Janus nanoplatelets using the Pickering emulsion method (**Nanomaterials 11**, 2797 (2021).

In the field of macromolecular soft matter, we have continued to study liquid-crystal elastomers. We described the synthesis of polydomain magnetic liquid-crystal elastomers, which is based on chemically bonding functionalised magnetic nanoparticles to the elastomer. This significantly enhances the response of the elastomer to the applied external magnetic field. We measured magnetic hystereses of the resulting polydomain samples in both low and high fields and identified two underlying mechanisms: particle reorientation and flipping of the magnetic moment within a single nanoparticle. We observed coupling between the mechanical stretching and magnetisation of the sample and found that the magnetisation, which occurs as a result of stretching, is almost equal to the magnetisation, which occurs under the influence of an external magnetic field. The results of our research have been published in **Liquid Crystals**, 48, 1815 (2021).

Biomedical optics

We have continued with development of innovative optical techniques for the non-invasive characterization of biological tissues and organs. By combining diffuse reflectance spectroscopy (DRS) and pulsed photo-thermal radiometry (PPTR; time-resolved measurements of laser-induced mid-infrared emission) with a dedicated numerical model of light transport in strongly scattering multi-layer structures, we have enabled an assessment of several physiologically relevant parameters of human skin *in vivo* (e.g., the contents of melanin and blood, together with its oxygen saturation level, in different skin layers). The described methodology was augmented and applied to the characterization of laser tattoo removal and longitudinal monitoring of traumatic bruises in human volunteers. Such methodology could enable future development of more accurate bruise aging methodology for forensic investigations. (**Sensors 21, 302, 2021**)

In collaboration with Department for Materials Synthesis (IJS), we studied inorganic nanoparticles which exhibit upconversion fluorescence (e.g., $NaYF_4$:Yb^{3+},Er^{3+}). Such nanoparticles have a great potential for diagnostic imaging in medicine and cell-targeted therapy. Most recently, we have focused on the development of phosphonate coatings, which improve their chemical stability under physiological conditions and thus minimize cytotoxicity, while at the same time preserving or even enhancing the upconversion fluorescence. (**Dalton Trans. 50**, 6588, 2021)

In a dedicated numerical simulation, based on the Monte Carlo modelling of light transport in multiple scattering regime, we have replicated measurements of diffuse reflectance using an integrating sphere (IS). The aim of the study was to assess the validity of time reversal symmetry, which is implicitly assumed in functioning of all commercial spectrometers using the IS, and test the strategies for minimization of the related artifacts in analyses of such measurements. (**Master thesis, FMF**, 2021)

> **Our unique methodology for non-invasive characterization of human skin in vivo could enable development of a bruise-ageing methodology, which would benefit forensic investigations.**
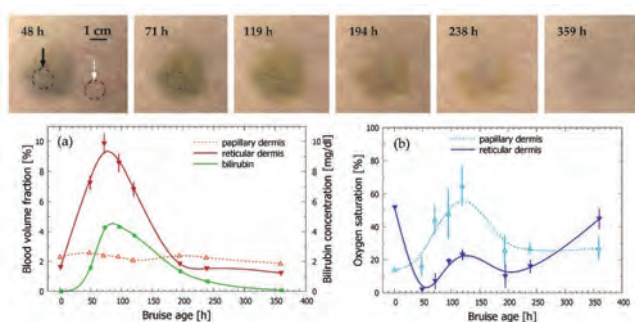
Figure 8: Top: Photographs of a bruise in human volunteer at different times after the injury. Bottom: (a) Time evolutions of bruise model parameters as assessed from measurements in the same bruise: volume fractions of blood in the papillary and reticular dermis, bilirubin concentration, and (b) the corresponding blood oxygenation levels.

Microfluidics

Microfluidics research has been carried out in close collaboration with the Laboratory for Experimental Soft Matter at the Faculty of Mathematics and Physics of the University of Ljubljana and, more recently, also with industrial pharmaceutical partners.

The year started by publishing the results of our research on the analysis of flow in microfluidic channels in **IEEE Sensors Journal, 21, 5871 (2021)**. We described a new type of microfluidic flow sensor, where the velocity measurements are not done on the fluid sample itself but on a second, immiscible fluid in contact with the sample. By monitoring the motion of the tracer particles in the side cavities, we have determined the characteristic parameters of the flows and shown a linear relationship with the fluid velocity over a wide range of measured velocities.

Another broad area of research is carried out in collaboration with pharmaceutical partners. We focus on studying particle dynamics, adsorption and aggregation in liquids and at their phase boundaries. We have used Brewster angle microscopy (BAM) to observe the adsorption dynamics of protein films at the water-air interface and to determine the rate of reconstitution of the films after abrupt rupture as a function of protein concentration. Additionally, protein films were damaged in a controlled manner and the resulting aggregates were analysed. We studied the dependence of the reconstitution and aggregation on the concentration of surfactant molecules. We found that the threshold concentrations for protein-film formation and protein aggregation are significantly lower than the critical micellar surfactant concentration. The work was included in a successfully defended master's thesis at the FMF.

> **In collaboration with industrial partners, we studied the formation of protein films at the water-air interface and measured the rate of their reconstitution after abrupt rupture and aggregate formation in the solution.**

Some outstanding publications in the past year

1. Mihailović, Dragan, Svetin, Damjan, Vaskivskyi, Igor, Lipovšek, Benjamin, Mraz, Anže. Ultrafast non-thermal and thermal switching in charge configuration memory devices based on 1T–TaS21T–TaS2. Applied physics letters, ISSN 0003-6951. [Print ed.], [in press] 2021, 16 str., doi: 10.1063/5.0052311. [COBISS.SI-ID 69786371]

2. Vaskivskyi, Igor, et al. Element-specific magnetization dynamics in Co-Pt alloys Induced by strong optical excitation : published as part of The Journal of Physical Chemistry virtual special issue %D. D. Sarma

Festschrift%. The journal of physical chemistry. C, Nanomaterials and interfaces, ISSN 1932-7447. [Print ed.], 2021, vol. 125, no. 21, str. 11714-11721, doi: 10.1021/acs.jpcc.1c02311. [COBISS.SI-ID 71606787]

3. Zhang, Renyun, Hummelgård, Magnus, Örtegren, Jonas, Olsen, Martin, Andersson, Henrik, Yang, Ya, Wang, Zhong-Lin, Olin, Håkan, Šutar, Petra, Mihailović, Dragan. All-inorganic triboelectric nanogenerators based on Mo6S3I6Mo6S3I6 and indium tin oxide. Nano energy, ISSN 2211-2855, [in press] 2021, 16 str., doi: 10.1016/j.nanoen.2021.106363. [COBISS.SI-ID 71502595]

4. Ravnik, Jan, Diego, Michele, Gerasimenko, Yaroslav, Vaskivskyi, Yevhenii, Mertelj, Tomaž, Vodeb, Jaka, Mihailović, Dragan. A time-domain phase diagram of metastable states in a charge-ordered quantum material. Nature communications, ISSN 2041-1723, 2021, vol. 12, str. 2323-1-2323-8, doi: 10.1038/s41467-021-2264. [COBISS.SI-ID 62665219]

5. Ravnik, Jan, Vaskivskyi, Yevhenii, Vodeb, Jaka, Aupič, Polona, Vaskivskyi, Igor, Golež, Denis, Gerasimenko, Yaroslav, Kabanov, Viktor V., Mihailović, Dragan. Quantum billiards with correlated electrons confined in triangular transition metal dichalcogenide monolayer nanostructures. Nature communications, ISSN 2041-1723, 2021, vol. 12, no. 1, str. 3793-1-3793-8, doi: 10.1038/s41467-021-24073-0. [COBISS.SI-ID 69789955]

6. Naseska, Mimoza, Šutar, Petra, Vaskivskyi, Yevhenii, Vaskivskyi, Igor, Vengust, Damjan, Svetin, Damjan, Kabanov, Viktor V., Mihailović, Dragan, Mertelj, Tomaž. First-order kinetics bottleneck during photoinduced ultrafast insulator-metal transition in 3D orbitally-driven Peierls insulator CuIr2S4CuIr2S4. New journal of physics, ISSN 1367-2630. [Online ed.], 2021, vol. 23, str. 053023-1-053023-10, doi: 10.1088/1367-2630/abf86d. [COBISS.SI-ID 77920003]

7. Pokharel, A. R., Agustsson, S. Y., Kabanov, Viktor V., Iga, F., Takabatake, T., Okamura, H., Demšar, Jure. Robust hybridization gap in the Kondo insulator YbB12YbB12 probed by femtosecond optical spectroscopy. Physical review. B, ISSN 2469-9950, 2021, vol. 103, vol. 11, str. 115134-1-115134-7, doi: 10.1103/PhysRevB.103.115134. [COBISS.SI-ID 56601091]

8. Toda, Yasnori, Tsuchiya, S., Oda, Migaku, Kurosawa, T., Katsumata, S., Naseska, Mimoza, Mertelj, Tomaž, Mihailović, Dragan. Ultrafast transient reflectivity measurements of optimally doped Bi2+xSr2−xCaCu2O8+δBi2+xSr2−xCaCu2O8+δ with disorder. Physical review. B, ISSN 2469-9950, 2021, vol. 104, no. 9, str. 094507-1-094507-9, doi: 10.1103/PhysRevB.104.094507. [COBISS.SI-ID 77929219]

9. Malik, R. S., Vaskivskyi, Igor, et al. Ultrafast magnetization dynamics in the half-metallic Heusler alloy Co2FeAlCo2FeAl. Physical review. B, ISSN 2469-9950, 2021, vol. 104, no. 10, str. L100408-1-L100408-6, doi: 10.1103/PhysRevB.104.L100408. [COBISS.SI-ID 83475971]

10. Tsuchiya, S., Taniguchi, Hiromi, Yamada, J., Toda, Yasnori, Mihailović, Dragan, Mertelj, Tomaž. Ultrafast dynamics of Mott-state quench and formation in strongly correlated BEDT-TTF molecular conductors observed by three-pulse pump-probe spectroscopy. Physical review. B, ISSN 2469-9950, 2021, vol. 104, no. 11, str. 115152-1-115152-6, doi: 10.1103/PhysRevB.104.115152. [COBISS.SI-ID 77907459]

11. Dasireddy, Venkata D. B. C., Vengust, Damjan, Likozar, Blaž, Kovač, Janez, Mrzel, Aleš. Production of syngas by CO2CO2reduction through Reverse Water-Gas Shift (RWGS) over catalytically-active molybdenum-based carbide, nitride and composite nanowire. Renewable energy, ISSN 0960-1481. [Print ed.], 2021, vol. 176, str. 251-261, doi: 10.1016/j.renene.2021.05.051. [COBISS.SI-ID 70734595]

Awards and Appointments

1. Prof. Martin Čopič: Winner of the "Blinc" award for the year 2021
2. Anže Mraz: Winner of the "Fernando Tommasini" award for the most comprehensible talk at the COROSSANO 2021 workshop
3. Aleš Mrzel and Damjan Vengust: Winners of bronze medal of ARCA 2021 award: Method for the synthesis of metal molybdates and tungstates from molybdenum and tungsten carbides and nitrides; National and University Library in Zagreb, Croatia, 14-16 October 2021

Organization of conferences, congresses and meetings

1. Nonequilibrium Quantum Workshop: Dynamics and Ergodicity of Complex Quantum Systems, Krvavec, Slovenija, 12–16 December 2021
2. 18th International Conference on Ferroelectric Liquid Crystals, Polarity and Chirality in Soft Matter, September 6 – 10, 2021, IJS, Slovenia

Patent granted

1. Nejc Lukač, Matjaž Lukač, Matija Jezeršek, Peter Gregorčič, Cleaning system, EP3510961 (B1), European Patent Office, 09. 06. 2021.

INTERNATIONAL PROJECTS

1. COST CA16101; MULTI-modal Imaging of FOREnsic SciEnce Evidence - tools for Forensic Science
   Prof. Boris Majaron
   Cost Office
2. COST CA16218; Nanoscale Coherent Hybrid Devices for Superconducting Quantum Technologies
   Prof. Viktor Kabanov
   Cost Association Aisbl
3. COST CA17123; MAGNETOFON; Ultrafast Opto-Magneto-Electronics for Non-Dissipative Information Technology
   Prof. Dragan Dragoljub Mihailović
   Cost Association Aisbl
4. COST CA17140 - Nano2Clinic; Cancer Nanomedicine - From the Bench to the Bedside
   Prof. Boris Majaron
   Cost Association Aisbl
5. COST CA20129; Multiscale Irradiation and Chemisty Driven Processes and Related Technologies
   dr. Lea Spindler
   Cost Association Aisbl
6. COST-CA17123;COST-CA17123; Ultrafest opto-magneto-electronics for non-dissipative information technology – MAGNETOFON
   Asst. Prof. Tomaž Mertelj
   Cost Association Aisbl
7. H2020 - INTERFAST; Gated INTERfaces for FAST information processing
   Asst. Prof. Tomaž Mertelj
   European Commission
8. H2020 - MAGNELIQ; A Magneto-Electric Liquid - Better Sensing
   Asst. Prof. Alenka Mertelj
   European Commission
9. Liquid Crystalline Properties of Guanosine-Rich DNA and RNA Oligonucleotides
   Prof. Irena Drevenšek Olenik
   Slovenian Research Agency
10. Microstructuring of Liquid Crystals and Light Wave Manipulation by Photorefractive Materials
    Prof. Irena Drevenšek Olenik
    Slovenian Research Agency
11. Studies of Structure and Dynamics of Liquid Magnets by SAXS and SANS
    Asst. Prof. Alenka Mertelj
    Slovenian Research Agency
12. Tunable Optical Diffractive Structures from Liquid Crystalline Materials
    Prof. Irena Drevenšek Olenik
    Slovenian Research Agency
13. Novel Liquid Crystalline Materials for Application in Diffractive Optical Elements
    Prof. Irena Drevenšek Olenik
    Slovenian Research Agency
14. Stretchable lasers

dr. Luka Cmok
Slovenian Research Agency

RESEARCH PROGRAMMES

1. Medical physics
   Dr. Matija Milanič
2. Light and Matter
   Prof. Irena Drevenšek Olenik
3. Dynamics of complex nano-systems
   Prof. Dragan Dragoljub Mihailović

R & D GRANTS AND CONTRACTS

1. Methods and materials for photoalignment templates for chiral liquid crystal lenses and photonic components
   Prof. Irena Drevenšek Olenik
2. Probing spin states near the surface of quantum spin materials
   Petra Šutar
3. Electrically tunable ferromagnetic liquids
   Dr. Alenka Mertelj
4. Phase transitions in systems of nucleotide repeat expansions associated with neurodegenerative diseases
   Prof. Irena Drevenšek Olenik
5. Mesoscopic Quantum Metastability
   Prof. Dragan Dragoljub Mihailović
6. Multi-scale modeling of non-equilibrium quantum materials
   Dr. Denis Golež
7. Liquid Magnets: fundamental studies of ferromagnetic order in liquids
   Dr. Nerea Sebastian Ugarteche
8. Surface-selective hybridization technology for magneto-electric hybrids
   Asst. Prof. Alenka Mertelj
9. Magneto Responsive Surfaces for Manipulation of Light and Liquids
   Prof. Irena Drevenšek Olenik
10. Exploitation of the magneto-mechanical effect in the treatment of neurodegenerative diseases
    Asst. Prof. Alenka Mertelj
11. Single-flux-quantum controlled charge configurational memory (CCM) devices
    Prof. Dragan Dragoljub Mihailović
12. CMEM: Ultrafast all-electronic charge density wave memory for next generation computing
    Dr. Igor Vaskivskyi
    Ministry of Education, Science and Sport
13. 18th International Conference on Ferroelectric Liquid Crystals (FLC 2021), Ljubljana, Slovenia, held from 6th to 10th of September 2021
    Asst. Prof. Alenka Mertelj

VISITORS FROM ABROAD

1. Dipl. ing. Inna Belyaeva, Faculty of Electrical Engineering and Information Technology, OTH Regensburg, Germany, 31st of May to 5th of June 2021
2. Dr Emil S.Bozin, Brookhaven National Laboratorium, USA, 21st of June to 23rd of June 2021
3. Dr Rinat Mamin, Zavoisky Physical-Technical Inst. of FIC KazanSC, Kazan, Russia, 19th of July to 19th of August 2021
4. Mag.Dejan Bošnjaković, Faculty of Electrical Engineering, Computer Science and Information Technology Osijek, Croatia, 19th of July to 23rd of July 2021
5. Dr Andrei Shumilin, Ioffe Institute, 26 Politekhnicheskaya, St.Petersburg, Russia, 29th of July to 29th of August 2021
6. Dr Mikhail Chamonine, Faculty of Electrical Engineering and Information Technology, OTH Regensburg, Germany, 30th of August to 6th of September 2021
7. Prof. Eremin Alexey, 5th of September to 11th of September 2021 (FLC conference)
8. Prof. Dr Nemanja Trišović, 12th of September to 17th of September 2021
9. Mag. Luka Matović. 12th of September to 17th of September 2021
10. Ph.D. Marcell Tibor Máthé, Wigner Research Centre for Physics, Budapest, Hungary, 26th of September to 24th of October 2021 and 8th of November to 4th of December 2021
11. Dr Virginie Coda-Bouchot, Université de Lorraine et CentraleSupélec, Metz, France, 23rd of October to 30th of October 2021
12. Dr Patrycja Łydżba, Wroclaw University of Science and Technology, 11th of December to 12th of December 2021 (NQW)
13. Dr Giuliano Chiriaco, The Abdus Salam International Centre for Theoretical Physics, 11th of December to 12th of December 2021(NQW)

STAFF

Researchers
1. Dr. Steven Daniel Conradson
2. Prof. Irena Drevenšek Olenik*
3. Dr. Denis Golež
4. Prof. Viktor Kabanov
5. Dr. Matjaž Lukač*
6. Prof. Boris Majaron
7. Asst. Prof. Alenka Mertelj
8. Asst. Prof. Tomaž Mertelj
9. **Prof. Dragan Dragoljub Mihailović**, Head
10. Asst. Prof. Matija Milanič*
11. Dr. Aleš Mrzel
12. Asst. Prof. Natan Osterman*
13. Dr. Nerea Sebastian Ugarteche
14. Asst. Prof. Lea Spindler*
15. Dr. Mojca Vilfan
Postdoctoral associates
16. Dr. Yelyzaveta Chernolevska

17. Dr. Luka Cmok
18. Dr. Andrej Petelin
19. Dr. Igor Vaskivskyi
20. Dr. Jaka Vodeb
Postgraduates
21. Neža Golmajer Zima, B. Sc.
22. Žiga Gregorin, B. Sc.
23. Patricija Hribar Boštjančič, B. Sc.
24. Gregor Jecl, B. Sc.
25. Andrej Kranjec, B. Sc.
26. Matija Lovšin, B. Sc.
27. Anže Mraz, B. Sc.
28. Mimoza Naseska, B. Sc.
29. Ankita Sarkar, M. Sc.

30. Yevhenii Vaskivskyi, M. Sc.
31. Rok Venturini, B. Sc.
Technical officers
32. Davor Grabnar, B. Sc.
33. Peter Medle Rupnik, B. Sc.
34. Damjan Svetin, B. Sc.
35. Petra Šutar, B. Sc.
36. Damjan Vengust, B. Sc.
Technical and administrative staff
37. Ula Groznik, B. Sc.
38. Martina Knavs, B. Sc.
39. Barbara Paternoster, B. Sc.

Note:
* part-time JSI member

BIBLIOGRAPHY

Original Article

1. Matjaž Ličen, Stefano Masiero, Silvia Pieraccini, Irena Drevenšek-Olenik, "Reversible photoisomerization in thin surface films from azo-functionalized guanosine derivatives", *ACS omega*, 2021, **6**, 23, 15421-15430.
2. Živa Marinko, Luka Suhadolnik, Barbara Šetina, Vid Simon Šelih, Boris Majaron, Janez Kovač, Miran Čeh, "Toward a flexible and efficient TiO_2 photocatalyst immobilized on a titanium foil", *ACS omega*, 2021, **6**, 36, 23233-23242.
3. Gaia Kravanja, Inna A. Belyaeva, Luka Hribar, Irena Drevenšek-Olenik, Matija Jezeršek, Mikhail Shamonin, "Tunable drop splashing on magnetoactive elastomers", *Advanced materials interfaces*, 2021, **8**, 11, 2100235.
4. Dragan Mihailović, Damjan Svetin, Igor Vaskivskyi, Rok Venturini, Benjamin Lipovšek, Anže Mraz, "Ultrafast non-thermal and thermal switching in charge configuration memory devices based on $1T-TaS_2$", *Applied physics letters*, 2021, **119**, 013106.
5. Jure Košir, Daniele Vella, Matjaž Lukač, Matija Jezeršek, "Towards personalized and versatile monitoring of temperature fields within heterogeneous tissues during laser therapies", *Biomedical optics express*, 2021, **12**, 7, 4530-4543.
6. Damjan Vengust, Boštjan Jančar, Tilen Sever, Andreja Šestan, Vid Bobnar, Zdravko Kutnjak, Nina Daneu, Danilo Suvorov, Matjaž Spreitzer, "Improved environmental stability of thermoelectric ceramics based on intergrowths of $Ca_3Co_4O_9-Na_{0.75}CoO_2$", *Ceramics international*, 2021, **47**, 8, 11687-11693.
7. Manal Benyoussef, Moneim Zannen, Jamal Belhadi, Bouchaib Manoun, Zdravko Kutnjak, Damjan Vengust, Matjaž Spreitzer, Mimoun El Marssi, Abdelilah Lahmar, "Structural, dielectric, and ferroelectric properties of $Na_{0.5}(Bi_{1-x}Nd_x)_{0.5}TiO_3$ ceramics for energy storage and electrocaloric application", *Ceramics international*, 2021, **47**, 18, 26539-26551.
8. Zouhair Hanani *et al.* (14 authors), "Morphogenesis mechanisms in the hydrothermal growth of lead-free BCZT nanostructured multipods", *CrystEngComm*, 2021, **23**, 30, 5249-5256.
9. Maša Vozlič, Tina Černič, Sašo Gyergyek, Boris Majaron, Maja Ponikvar-Svet, Uliana Kostiv, Daniel Horák, Darja Lisjak, "Formation of phosphonate coatings for the improved chemical stability of upconverting nanoparticles under physiological conditions", *Dalton transactions*, 2021, **50**, 19, 6588-6597.
10. Nika Mlinarič, Natan Osterman, "Proof-of-concept experiment of microfluidic flow sensor based on microcavity-secondary-flow observation", *IEEE sensors journal*, 2021, **21**, 5, 5871-5878.
11. Anže Mraz, Igor Vaskivskyi, Rok Venturini, Damjan Svetin, Yelyzaveta Chernolevska, Dragan Mihailović, "Charge Configuration Memory (CCM) device – a novel approach to memory", *Informacije MIDEM*, 2021, **51**, 3, 157-167.
12. Melani Potrč, Nerea Sebastián, Miha Škarabot, Irena Drevenšek-Olenik, Lea Spindler, "Supramolecular polymorphism of $(G_4C_2)_n$ repeats associated with ALS and FTD", *International journal of molecular sciences*, 2021, **22**, 9, 4532.
13. Daniel Ząbek, Andrzej Grzebielec, Luka Cmok, Patricija Hribar, Alenka Mertelj, "Experimental analysis of the stability of ferrofluids based on Iron Oxide powder", *Inżynieria Bezpieczeństwa Obiektów Antropogenicznych*, 2021, **2**, 1-6.
14. Daniel Duffy, Luka Cmok, John S. Biggins, Abhijeet Krishna, Carl D. Modes, Mustafa K. Abdelrahman, Muhammad Javed, Taylor H. Ware, Feng Fang, Mark Warner, "Shape programming lines of concentrated Gaussian curvature", *Journal of applied physics*, 2021, **129**, 22, 224701.
15. Luka Rogelj, Urban Simončič, Tadej Tomanič, Matija Jezeršek, Urban Pavlovčič, Jošt Stergar, Matija Milanič, "Effect of curvature correction on parameters extracted from hyperspectral images", *Journal of biomedical optics*, 2021, **26**, 9, 096003.
16. Igor Vaskivskyi *et al.* (13 authors), "Element-specific magnetization dynamics in Co-Pt alloys Induced by strong optical excitation", *The journal of physical chemistry. C, Nanomaterials and interfaces*, 2021, **125**, 21, 11714-11721.
17. Matija Jezeršek, Nejc Lukač, Matjaž Lukač, "Measurement of simulated debris removal rates in an artificial root canal to optimize laser-activated irrigation parameters", *Lasers in surgery and medicine*, 2021, **53**, 3, 411-417.
18. Matjaž Lukač, Giovanni Olivi, Mihnea Constantin, Nejc Lukač, Matija Jezeršek, "Determination of optimal separation times for dual-pulse SWEEPS laser-assisted irrigation in different endodontic access cavities", *Lasers in surgery and medicine*, 2021, **53**, 7, 998-1004.
19. Matjaž Lukač, Anže Zorman, Nejc Lukač, Tadej Perhavec, Blaž Tašič Muc, "Characteristics of non-ablative resurfacing of soft tissues by repetitive Er:YAG laser pulse irradiation", *Lasers in surgery and medicine*, 2021, **53**, 9, 1266–1278.
20. Luka Cmok, Mojca Vilfan, Sašo Gyergyek, Martin Čopič, "Magnetic polydomain liquid crystal elastomers - synthesis and characterisation", *Liquid crystals*, 2021, **48**, 13, 1815-1826.
21. Nerea Sebastián, Richard J. Mandle, Andrej Petelin, Alexey Eremin, Alenka Mertelj, "Electrooptics of mm-scale polar domains in the ferroelectric nematic phase", *Liquid crystals*, 2021, **48**, 14, 2055-2071.
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SHORT ARTICLE

1. Denis Golež, Zhiyuan Sun, "A compact device sustains a fluid of bosons", *Nature*, 2021, **598**, 7882, 571-572.

PUBLISHED CONFERENCE CONTRIBUTION

1. Patrick Seleš, Žiga Lipovšek, Martina Kocijan, Tina Radošević, Damjan Vengust, Matejka Podlogar, "Synthesis of ZnO powders with different morphologies for photocatalytic degradation", In: *56th International Conference on Microelectronics, Devices and Materials & the Workshop on Personal Sensors for Remote Health Care Monitoring, 22-24 September 2021, Ljubljana, Slovenia*, Proceedings, MIDEM, 2021, 35-42.

2. Jošt Stergar, Katja Lakota, Martina Perše, Matija Tomšič, Matija Milanič, "Vasculature based biomarkers and segmentation from hyperspectral images of murine peritonitis model", In: *European Conferences on Biomedical Optics 2021, ECBO, 20-24 June 2021, Munich, Germany*, Optica, 2021, ETu1A.6.

3. Tadej Tomanič, Luka Rogelj, Matija Milanič, "GPU-accelerated inverse adding-doubling algorithm for analysis of skin hyperspectral images", In: *European Conferences on Biomedical Optics 2021, ECBO, 20-24 June 2021, Munich, Germany*, Optica, 2021, EW4A37.

PATENT

1. Nejc Lukač, Matjaž Lukač, Matija Jezeršek, Peter Gregorčič, *Cleaning system*, EP3510961 (B1), European Patent Office, 09. 06. 2021.

THESES AND MENTORING

1. Jošt Stergar, *Combined hyperspectral imaging of macroscopic and microscopic samples for tissue optical and structural properties evaluation:* doctoral dissertation, Ljubljana, 2021 (mentor Matija Milanič).

2. Jaka Vodeb, *Configurational electronic states in layered trasition metal dichalcogenides:* doctoral dissertation, Ljubljana, 2021 (mentor Dragan Mihailović; co-mentor Viktor Kabanov).

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 in fusion reactors*
- *physics of semiconductors*
- *medical physics*

Head:
Prof. Luka Snoj

The main objective of the project entitled Stability of nuclear reactors in load-follow mode of operation, which started in 2020, is to the examine restrictions of the nuclear-power-plant load-follow operation on the nuclear aspects of the reactor core and nuclear fuel and provide effective solutions for the plant operator regarding how to optimize the plant's operation. In 2020 communications with all partners, including the industry partners, were established. Additionally, the research activities on all the work packages were started and were proceeding according to the envisioned time schedule. The first research results are expected in 2021.

The objective of the proposed research entitled Sensitivity of nuclear reactor physical parameters to thermal nuclear data is to generate thermal neutron scattering cross-sections and corresponding covariance data in a rigorous manner that is from first principles, by employing state-of-the-art atomistic simulations, which rely on density functional theory in combination with lattice or molecular dynamics calculations. As part of the project, activities regarding atomistic simulations for the needs of producing thermal scattering data have begun. Additionally, communication channels have been established with North Carolina State University, whose experts will contribute the know-how that will result in a successful start to the project. The work on the project is proceeding according to the time schedule envisioned in the project's proposal. The first calculations of the selected benchmark test cases with the new thermal scattering data were carried out before the end of 2021.

The objective of the proposed research entitled Advances in Thermal Scattering Law Analysis is to generate thermal neutron scattering cross-sections for materials that have not yet been investigated, such as uranium hydride fuel, as well as conventional moderators (such as polyethylene, Lucite, Teflon and graphite). In addition to the thermal neutron scattering cross-sections the corresponding covariance data need to be obtained. A process for generating thermal neutron scattering cross-sections in a form for use in the Monte Carlo code from a predetermined density of states was established and tested. The procedure was performed using NJOY modules (LEAPR, RECONR, BROADR, THERMR and ACER modules). The obtained data are currently in the process of validation with experimental values. In the next year, activities for the generation of density of states for various materials will begin.

The primary objective of the European TOURR project, which started in 2020, is to develop a strategy for Research Reactors in Europe and to prepare the ground for its implementation. This strategic goal can be divided into specific objectives: Assessment of the current status of the European RR fleet, including plans for upgrade; evaluation of urgent EU needs; developing tools for the optimal use of the RR fleet and rising awareness among decision makers on the (future) role of RRs. The JSI is leading the first objective, whereas we are responsible for gathering information on the status and plans of the fleet of European research reactors. Additionally, we are involved in the strategy for the dissemination of the results.

Researchers of the Reactor Physics Department provided technical support for the safe operation of the Krško nuclear power plant (NPP) in 2021. We have independently performed nuclear-core design calculations for the fuel cycle 32 and the start-up tests for the new fuel cycle. An independent evaluation of the reload safety evaluation for the cycle 32 has been performed. In addition, the expertise and calculational support for the future dry storage of spent nuclear fuel was provided. The focus was on a sensitivity analysis of the main parameters for the spent-fuel characterization.

In 2021 our team worked on a project to support the NEK power plant in designing and implementing a dry-storage repository for spent fuel. We conducted studies and made improvements to increase the accuracy of the spent-fuel source term and reduce uncertainty in future core design calculations. We have established a workflow for the generation of perturbed WIMS libraries for the purpose of using them in uncertainty propagation and sensitivity-analysis studies, including a method for simultaneous sampling.

In the framework of the international project E-SiCure2 - Enhancing security at borders and ports, conducted as an international collaboration and funded by the NATO Science for Peace and Security programme, we initiated

the development of silicon carbide (SiC) based detectors of multiple radiation types. The research activities are being carried out on the basis of the results of a previous project – E-SiCure (2016-2019). The goal is the development of pixelized detectors that will enable the simultaneous detection of thermal and fast neutrons, charged particles as well as X and gamma radiation. We have carried out an intensive testing campaign of prototype detectors using alpha particle and neutron sources, and initiated simulations of the detector response for different converter materials, enabling sensitivity to thermal and fast neutrons. The results of the computational search for new converter materials were presented in a contribution to the NENE 2021 conference, where the work received the reward for best conference poster.

We continued our collaboration with the Rolls-Royce Civil Nuclear SAS company (Meylan, France) on the topic of the experimental testing of detectors for nuclear instrumentation at the JSI TRIGA reactor. In 2021 we carried out a 3-day experimental testing campaign.

In 2021 we continued work in the framework of the European project EURAD, in WP3 CORI – cement-organic interactions between radionuclides and WP8 SFC – spent fuel characterization. In WP3 of the CORI programme for radioactive-waste management we investigated interactions between cement, organic molecules and radionuclides in the context of the safe disposal of low- and intermediate-level radioactive waste. We performed a study on the radiolysis of superplasticicators through gamma irradiations at the JSI TRIGA reactor. In WP8 we performed several detailed calculations of the decay heat and photon/neutron source term of spent fuel assemblies originating from PWR reactors. The focus was on sensitivity and uncertainty analyses with the use of different codes and models.

Figure 1: Energy spectrum of alpha particles coming from a sample of americium 241 after neutron irradiation. The two peaks visible correspond to the americium 241 and its activation product curium 242.

In 2021 we continued our collaboration efforts in the framework of the European project ENEEP - European Nuclear Experimental Educational Platform. The aim of the project is to establish a platform at the European level, enabling experimental education activities in the field of nuclear science and engineering for students at all educational levels and young professionals. The project is being carried out as a collaboration with STU (Slovakia), CTU (Czech Republic), ATI (Austria) and BME (Hungary). In 2021 we led activities in work package 4 of the project, which will lead to the establishment of the platform itself.

In collaboration with colleagues from CEA Cadarache we continued with research on the feasibility of the use of reactor pulse mode for specific applications, e.g., for nuclear instrumentation testing at very high neutron-flux levels, i.e., up to 1016 n cm^{-2} s^{-1}, achievable only in this operation mode. This requires a capability for online neutron-flux measurements in challenging conditions, as the neutron flux level changes by 6–7 orders of magnitude in a few ms. In 2021 a series of test measurements using miniature fission chambers and the MONACO data-acquisition system developed at the CEA.

In 2021 in collaboration with colleagues from CEA Cadarache we continued activities in the framework of the project "Experimental Benchmark for validation of the modelling of neutron and gamma instrumentation". The aim of the project is to perform an exhaustive experimental campaign at the JSI TRIGA reactor in which the signals of several detector types will be measured (fission and ionization chambers, self-powered neutron detectors, activation measurements, thermoluminescent detectors), and the comparison of the experimental data with the results of simulations performed using the Monte Carlo method.

In collaboration with CEA Cadarache, we continued experimental activities in the framework of the project on [241]Am thermal neutron capture cross-section measurements. Measurements of [242]Am/[242]Cm activation were performed in the F-19 irradiation channel in the F-ring of the reactor core and the IC-40 irradiation channel in the graphite reflector of the JSI TRIGA reactor using low-activity [241]Am samples, produced at JSI. The activation measurement in the TRIGA central channel were partially analysed. From the measured activated sample activities, reaction rates were derived using full uncertainty propagation. A preliminary value of ~720 b was obtained for the thermal neutron capture cross-section in [241]Am. A full uncertainty propagation is planned for 2022. In 2022 we plan the analysis of the measurements in the graphite reflector and F-ring.

In 2021 the project "New inelastic scattering nuclear reactions for epithermal neutron dosimetry" started in collaboration with CEA Cadarache. The first goal of the project, to search for suitable (n,n') reactions for irradiation at the JSI TRIGA reactor, was achieved. The second goal, irradiation of standard materials and materials for activation via (n,n') reactions at the TRIGA reactor, is planned for 2022. The third goal, C/E comparison, is planned for the end of 2022 or for 2023.
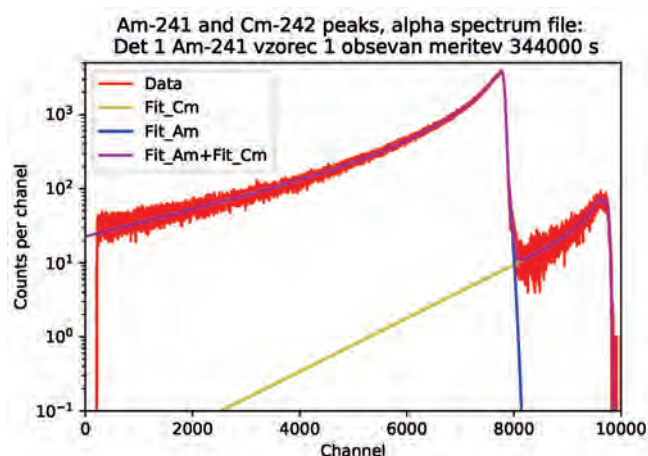
In 2021 we collaborated within the European SANDA project. The JSI contributes work in several different areas, including the use of programmes for sensitivity and uncertainty analysis, calculations of benchmark experiments and their use for the validation and improvement of nuclear data.

We continued an international collaboration led by the Swedish organizations Vattenfall, SKB and SSB in the field of spent PWR fuel characterization. In connection with the so-called "Blind Test", where the decay heat from PWR fuel assemblies was determined, a common publication summarising all the results was being finalised. A scientific paper is planned for publication in 2022.

In the scope of a collaboration with the International Atomic Energy Agency (IAEA) we participated in the CRP project "Spent Fuel Characterization". We contributed a sensitivity analysis of the irradiation parameters and the influence of different neutron cross-section libraries on the 16×16 spent-fuel characterization.

In collaboration with other departments at the JSI we have demonstrated that both gamma and electron-beam irradiation can be used for sterilization, provided that the respirators are recharged afterwards. Even though the FFRs are designed for single use, the pandemic crisis made it necessary to seek for emergency alternatives. This achievement won the Excellence in Science award from the ARRS.

Non-intermittent, low-carbon energy from nuclear or biofuels is integral to many strategies to achieve Carbon Budget Reduction targets. However, nuclear plants have high upfront costs and biodiesel manufacture produces waste glycerol with few secondary uses. Combining these technologies, to precipitate valuable feedstocks from waste glycerol using ionizing radiation, could diversify nuclear energy use whilst valorising the biodiesel waste. We demonstrated solketal (2,2-dimethyl-1,3-dioxolane-4-yl) and acetol (1-hydroxypropan-2-one) production is enhanced in selected aqueous glycerol-acetone mixtures with γ radiation.

Last year was important for the Laboratory for Plasma Physics as it represented the beginning of the new FP9 framework programme, where many projects inside the EUROfusion Consortium received new content and were redressed. We managed to maintain our presence in the MST tokamak experimental campaigns, which are now, together with the JET tokamak, running under the project name WPTE (Tokamak Exploitation). Due to the Covid-19 epidemics in 2021 we had to limit our contribution to simulations and the development of simulation models of the filamentary transport within the research task RT15. Our research was directed into divertor and main-chamber recycling as well as the influence of the filament size. We used computational resources obtained at the super computer HPC Marconi for these simulations and the work will continue in 2022. Because of the Covid-19 situation, our basic Enabling Research project with an international team titled "Emissive divertor" was extended into 2021. Due to that extension we were able to develop a coupled model of the emission from a divertor monoblock using a PIC code and a simple thermal model of the emitting surface. Furthermore, we have completed a successful validation and verification of our analytical model of the inverted sheath caused by high thermionic emission. The validation was performed using a PIC kinetic code, which provided us with new insights into the physical properties of such a sheath, but also revealed some inconsistencies in the code and the model. The latter will be the subject of our work in 2022. There is a new large project formed in the programmatic scheme of the EUROfusion Consortium called Theory, Simulation, Verification and Validation (TSVV) project. We became part of two development tasks within the TSVV, namely the development of kinetic and gyrokinetic codes and the development of divertor models for the future demonstrational fusion power plant DEMO. In the first task we work on the development of boundary conditions for gyrokinetic codes and in the second one we are involved in the modelling of the divertor plasma, the results of which will contribute to an understanding of such plasma and improve the predicative capabilities of the plasma behaviour in such a low-temperature divertor.

We have started work on the project for the design of the future fusion power plant DEMO in the field of neutronic calculations, activation, delayed heat and dose-rate calculations. Our task is to calculate the activation and delayed heat in divertor components for different times after the reactor shutdown. The irradiation scenario consists of about 5 years of continuous irradiation followed by several reactor pulses, at a fusion power of 2 GW. We are also involved in the review of the DEMO safety report with the aim of providing as many long-term recommendations as possible. Our group focuses on conventional hazard analysis and the quantification of radiation sources.

In 2021 we started our work on the project "Machine-learning-based optimization of fusion reactor neutronics performance". The work included the parametrisation of simpler models of tokamak that can be used in combination with optimisation algorithms. We also started to look for suitable optimisation algorithms for use with these models.

In 2021 the F8 team, in collaboration with colleagues from multiple European institutes, laboratories and universities, analysed results from experimental work on the Joint European Torus – JET tokamak, currently the largest operational fusion reactor. The majority of our work was dedicated to calculations of neutron field in various parts of the reactor and comparisons of these values with experimentally obtained values. We simulated detector responses for various plasma sources (DD, DT, TT) and evaluated the possibility of experimentally determining the neutron spectrum of the TT plasma source. Our most important results were comparisons of calculations and measurements for the neutron activation of samples during the C38-DD campaign at JET that were irradiated

in a long-term irradiation station (O-LTIS). The results showed excellent agreement between the calculated and experimentally determined activation of samples, which is a good starting point for similar future analyses in support of the future TT and DT campaigns at JET. Furthermore, in 2021 we also collaborated in development of the methodology for the simulation of gamma source and transport in tokamak JET. This work is done in support of the experimental work as gamma-ray measurements could potentially complement fusion-power measurements performed with neutron detectors.

Within the EUROfusion framework we continued an international collaboration in the field of fusion that stared more than 20 years ago, specifically on 21–22 March 2000 when Slovenia joined the European fusion program. In 2021 we contributed with an S/U analysis of 14 MeV neutron-shielding cases, including a new experiment at FNG in Frascati called WCLL (Water Cooled Lithium Lead). The benchmark experiment was modelled using the Monte Carlo codes ADVANTG/MCNP for particle transport and SANDY for sensitivity and uncertainty analysis of nuclear data. In addition, work on fusion-relevant water activation at the TRIGA reactor was continued.

We participated in the work of the Fusion Technology programme group, which started in January 2019. This programme group includes leading Slovenian experts in the field of fusion technologies and plasma physics from four departments of the Jožef Stefan Institute and two faculties of the University of Ljubljana. Four of the eleven researchers in this group come from the F8 department.

In 2021 we actively participated in the JET3-NEXP streaming benchmark experiment. The project ended in 2021 and is being continued as part of a new project entitled Preparation for ITER Operation (PrIO). We continued the
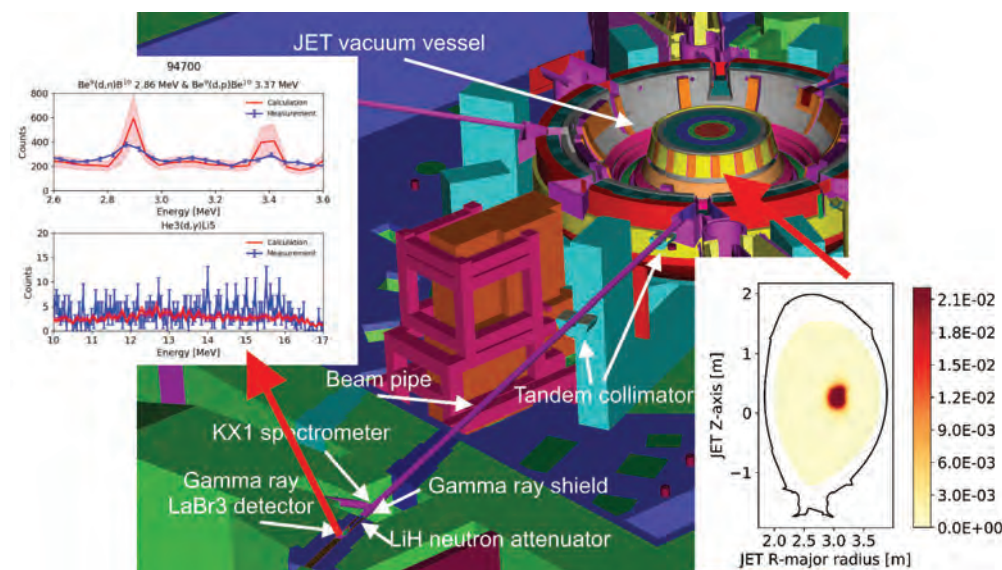

Figure 2: Comparison of calculated absolute fusion gamma-ray spectra and measurements for a detector position located 20 m from the plasma using a realistic Monte Carlo gamma-ray source. The agreement between calculations and measurements is excellent and unprecedented for the research field.

analysis of the experiments to determine neutron streaming performed using thermoluminescent detectors and activation foils. The simulation of the neutron fluence and reaction rates were conducted using hybrid (deterministic/Monte Carlo) transport codes for several experimental locations positioned in the tokamak building. This year the JSI also contributed a part of the final project report. The record DT experiments performed at JET at the end of 2021 will be analysed as part of the PrIO project in 2022.

In 2021 we continued our collaboration with the Culham Centre for Fusion Energy in the UK through the appointment of a post-doctoral researcher to a long-term secondment to tokamak JET. In 2021 the researcher continued in their role of TRANSP responsible officer, offering support to the experimental campaigns at the JET tokamak by performing plasma-transport analyses and in the roles of diagnostic coordinator and BEAST code inter-shot plasma expert, both in the control room of JET. We participated in the preparation and analysis of numerous experiments within the experimental campaigns using tritium and deuterium-tritium plasmas. In the scope of plasma-analysis support of experiments at JET using a mixture of D-3He fuel, we have measured and modelled the response of several neutron detectors through the coupling of TRANSP-DRESS-MCNP codes. We have shown that it is possible to detect the effects of fast ions on neutron spectrum anisotropy in externally heated plasmas using a combination of indium and aluminium activation foils, which has also been computationally validated. The collaboration ended in November 2021, as at that time the previous EUROfusion financing ended and a new one began, which does not include post-doctoral research at JET.

In the field of medical physics, specifically in the biomedical optics, we have continued the research started in the previous periods. We have based the work around hyperspectral microscopy. We have performed research on the microscopic structure and optical properties of tissue-mimicking phantoms. The results were compared with different analytical computations of scattering cross-sections and measurements using other modalities. We have developed novel contrasts and biomarkers for hyperspectral microscopy based on tissue structure that are able to classify subjects based on their disease state. These topics presented a significant part of the doctoral thesis of Jošt Stergar while opening new lines of the research for the future. Results were presented on international confer-

ences from the field. We have continued the close collaboration with the University of Rijeka and the University of Bologna, where we studied different machine-learning methods for the analysis of medical images and use of optical methods in the preservation of the cultural heritage. The latter included the development of an imaging system that enables the two-dimensional acquisition of infrared spectroscopy (FTIR) images and hyperspectral microscopy of different relevant samples.

In addition we continued our research in the field of positron emission tomography (PET) image analysis. We focused mainly on the use of PET imaging in neurology, in the differential diagnosis of neurodegenerative diseases. The use of FDG-PET imaging alone, combined with network analysis, has already been used in research for the differential diagnosis of parkinsonism and dementia. However, there is still an open question of what FDG-PET images can be used for network analysis and how many images are needed for a useful model. In our research we found that a sufficient number of reference images (at least 30 patients and 30 healthy controls) were required for a successful differential diagnosis. We also found that these images can have relatively poor resolution (in the range 12 to 15 mm FWHM).

As always in recent years, we closely collaborated with the University of Wisconsin - Madison. The groups continued with the tight organizational integration this year (regular Zoom weekly meetings, internal reviews of papers, etc.)

Awards and Appointments

1. Andrej Žohar: Best Poster Award, Bled, "30th International Conference Nuclear Energy for New Europe – NENE 2021", September 2021, poster "Silicon carbide neutron detector development computational support with MCNP"
2. Award of the Slovenian Research Agency (ARRS) for Research Activity of the Republic of Slovenia 'Excellent in Science 2021' in the category Technology, subcategory Energy for the work "Sterilization of polypropylene membranes of facepiece respirators by ionizing radiation" (doi.org/10.1016/j.memsci.2020.118756)

INTERNATIONAL PROJECTS

1. Irradiation Services for the Rolls-Royce Civil Nuclear SAS Company
   Dr. Vladimir Radulović
   Rolls-Royce Civil Nuclear Sas
2. E-SiCure2 - Enhancing Security at Borders and Ports
   Prof. Luka Snoj
   Nato - North Atlantic Treaty Organisation
3. Kinetic Approach to Modelling and Measurements in SOL of Tokamak; Network of Small and Medium Size Magnetic Confinement Fusion Devices for Fusion Research
   Dr. Jernej Kovačič
   IAEA - International Atomic Energy Agency
4. IAEA RC 24324 - Spent Fuel Characterization Uncertainties Due to Variations in Fuel Characteristics and Irradiation History; CRP T13018: Spent Fuel Characterization
   Asst. Prof. Marjan Kromar
   IAEA - International Atomic Energy Agency
5. H2020 - EURAD; European Joint Programme on Radioactive Waste Management
   Dr. Vladimir Radulović
   European Commission
6. H2020 - ENEEP; European Nuclear Experimental Educational Platform
   Dr. Vladimir Radulović
   European Commission
7. H2020 - SANDA; Supplying Accurate Nuclear Data for Energy and Non-Energy Applications
   Prof. Ivan Aleksander Kodeli
   European Commission
8. H2020 - ARIEL; Accelerator and Research Reactor Infrastructures for Education and Learning
   Prof. Ivan Aleksander Kodeli
   European Commission
9. H2020 - TOURR; Towards Optimized Use of Research Reactors in Europe
   Prof. Luka Snoj
   European Commission
10. H2020 - EUROfusion; Research Unit - Administration and Services RU – FU
    Prof. Luka Snoj
    European Commission
11. H2020 - EUROfusion; Enabling Research-2-FU
    Dr. Jernej Kovačič
    European Commission
12. H2020 - EUROfusion; Plasma Facing Components-1-IPH-FU, EUROfusion
    Dr. Jernej Kovačič
    European Commission
13. H2020 - EUROfusion; Exploitation of DT Operation for ITER-JET3-FU
    Prof. Luka Snoj
    European Commission
14. H2020 - EUROfusion; JET Campaigns-JET1-FU
    Dr. Žiga Štancar
    European Commission
15. H2020 - EUROfusion; PMI-PPPT-2-FU: Nuclear data
    Prof. Ivan Aleksander Kodeli
    European Commission
16. Multiphysics Validation of High Fidelity Modelling and Simulation for Nuclear Applications
    Dr. Vladimir Radulović
    Slovenian Research Agency
17. Use of Shielding Benchmarks for Nuclear Data Validation and Improvement
    Prof. Ivan Aleksander Kodeli
    Slovenian Research Agency
18. Optimization of Neutron Converting Components for Enhanced Performance of Silicon Carbide Based Neutron Detectors
    Prof. Luka Snoj
    Slovenian Research Agency
19. Steady-State and Transient Experimental Benchmark for Validation and Development of the TRAPID Neutronics Code Using the JSI TRIGA Mark-II Reactor
    Prof. Luka Snoj
    Slovenian Research Agency
20. Development of Multiphysics Tools for Plasma and Neutron Transport Calculations in Modern Fusion Devices
    Dr. Žiga Štancar
    Slovenian Research Agency
21. Steady-State and Transient Experimental Benchmark for Validation and Development of the TRAPID Neutronics Code Using the JSI TRIGA Mark-II Reactor
    Dr. Aljaž Čufar
    Slovenian Research Agency
22. HE - EUROfusion; WP08: DES-1,2_HE-FU
    Dr. Aljaž Čufar
    European Commission
23. HE - EUROfusion; WP19: SAE-1_HE-FU
    Domen Kotnik
    European Commission

24. HE - EUROfusion; WP10: BB_HE-FU
Dr. Gašper Žerovnik
European Commission
25. HE - EUROfusion; WP06: PrIO-5_HE-FU; WPPrio-ITERneutronics&Safety
Prof. Luka Snoj
European Commission
26. HE - EUROfusion; WP01: WPTE - Tokamak Exploitiat, HE - EUROfusion; WP01: WPTE-JET
Dr. Jernej Kovačič
European Commission
27. HE - EUROfusion; WP04: AC- TSVV-4,7_HE-FU
Dr. Jernej Kovačič
European Commission
28. HE - EUROfusion; WP25: PMU_HE-FU, RU-Mgmt-1_HE-FU
Prof. Luka Snoj
European Commission
29. HE - EUROfusion; WP24: TRED_HE-FU, EDU_HE-FU
Prof. Luka Snoj
European Commission

RESEARCH PROGRAMMES

1. Medical physics
Prof. Robert Jeraj
2. Reactor Physics
Prof. Luka Snoj
3. Fusion technologies
Prof. Igor Lengar

R&D GRANTS AND CONTRACTS

1. Contribution to the improvement of nuclear data for higly reliable reactor shielding calculations
Prof. Ivan Aleksander Kodeli
2. Absolute radiation measurements at very high neutron flux levels in reactor pulse mode
Prof. Igor Lengar
3. Electrocaloric elements for active cooling of electronic circuits
Prof. Luka Snoj
4. Advances in Thermal Scattering Law Analysis
Prof. Luka Snoj
5. Experimental Benchmark for validation of the modelling of neutron and gamma instrumentation
Dr. Vladimir Radulović
6. Sensitivity of nuclear reactor physical parameters to thermal nuclear data
Prof. Andrej Trkov
7. New inelastic scattering nuclear reactions for epithermal neutron dosimetry
Dr. Gašper Žerovnik

8. Stability of nuclear reactors in load follow mode of operation
Prof. Luka Snoj
9. Irradiations on the TRIGA Reactor
Prof. Luka Snoj
10. Neutron Transport and Criticality Calculations in Reactor Cores
Dr. Vladimir Radulović
Institut de Radioprotection et de Surete Nucleaire
11. Irradiations of FT-TIMS Capsule on the TRIGA Reactor for Years 2020-2022
Prof. Luka Snoj
Cea-commissariat A L' Energie Atomique Et Aux
12. Secondment – JET
Dr. Žiga Štancar
United Kingdom Atomic Energy Authority - Ukaea
13. SiC Campaign within the Frame of the Contract between CEA/AMU and FRAMATOME
Dr. Vladimir Radulović
Cea Saclay

NEW CONTRACTS

1. Assessment of ex-core power detector signal dependence on their positions
Prof. Luka Snoj
Krško Nuclear Power Plant
2. Independent Evaluation of the NPP Krško Cycle 32, Reload Safety Evaluation
Asst. Prof. Marjan Kromar
Krško Nuclear Power Plant
3. Reload Operational Core Analysis, Post Refuelling Nuclear Design Check Tests, PIS and KFSS Cycle Specific Data for Future Fuel Cycles (Cycle 31)
Asst. Prof. Marjan Kromar
Krško Nuclear Power Plant
4. Activities to support SFDS calculation and implementation
Prof. Luka Snoj
Krško Nuclear Power Plant
5. Optimization of storage in dry storage containers – SFDS
Asst. Prof. Marjan Kromar
Krško Nuclear Power Plant
6. Support for reviews and calculations in the SFDS project for 2020 and 2021
Prof. Luka Snoj
Krško Nuclear Power Plant
7. L2-2612 co-financing of L-project: Stability of nuclear reactors in load follow mode of operation
Prof. Luka Snoj
Gen Energija, d. o. o.
8. Reload Operational Core Analysis, Post Refuelling Nuclear Design Check Tests, PIS and KFSS Cycle Specific Data for Future Fuel Cycles (Cycle 32)
9. Asst. Prof. Marjan Kromar
Krško Nuclear Power Plant
10. NEK PSR3 Project Task „Safety Analyses"
Prof. Luka Snoj
Krško Nuclear Power Plant

VISITORS FROM ABROAD

1. Dr Loic Barbot, Dr Gregoire de Izarra, Commissariat a l'Energie Atomique – CEA / DER / SPESI / LDCI, Cadarache, France, 14.–16. 6. 2021
2. Dr Damien Fourmentel, Dr Hubert Carcreff, Commissariat a l'Energie Atomique – CEA, Cadarache, France, 19. 7.–23. 7. 2021
3. Dr Blaž Likozar and Mr. Anže Prašnikar, National Institute of Chemistry, Ljubljana, 13. 8. 2021
4. Branislav Vrban and Štefan Čerba, Slovak University of Technology in Bratislava, Bratislava, Slovakia, 6. 9.–9. 9. 2021
5. Valentin Valero, IM2NP Laboratory, University Aix-Marseille, France, 20. 9.–18. 12. 2021
6. Prof. Andreas Solders, prof. Dr Zsolt Elter, Uppsala University, Uppsala, Sweden, 27. 9.–1. 10. 2021
7. Prof. Piero Ravetto, Politecnico di Torino, Dipartimento Energia, NEMO Group, Torino, Italy, 18. 10.–21. 10. 2021
8. Mr. Bret Kugelmass and prof. Adam Zuckerman, Energy Impact Center, Washington DC, USA, 21. 10. 2021
9. Zalán Bata, Marcell Kégl, Dávid Korom, Levente Lovas, Budapesti Muszaki es Gazdasagtudomanyi Egyetem, Budapest, Hungary, 25. 10. 2021

10. Prof. Vladimir Demidov, West Virginia University, Morgantown, WV, USA, 29. 10. 2021–28. 10. 2022
11. Dr Damien Fourmentel and Dr Gregoire De Izarra, CEA Cadarache, France; Dr Laurent Ottaviani, University Aix-Marseille, France; Mr Patrick Konrad, Mr Heiko Jasper and Mr Patrick Weidenauer, Framatome, France, 2. 11.–5. 11. 2021
12. Mrs. Christelle Reynards Carette, Mr Adrien Volte and Mr Michel Carette, University Aix-Marseille, France, 8. 11.–12. 11. 2021
13. Dr Christophe Destouches, CEA Cadarache, France, 15. 11.–19. 11. 2021
14. Dr Elchin Huseynov, National Nuclear Research Centre, Baku, Azerbaijan, 19. 11.–27. 11. 2021
15. Dr Laurent Ottaviani, Institute Matériaux Microélectronique Nanosciences de Provence, University Aix-Marseille, France, 22. 11.–27. 11. 2021
16. Dr Loic Barbot and Dr Gregoire de Izarra, CEA, Cadarache, France, 6. 12.–10. 12. 2021
17. Mr. Danilo Bisiach, Mr. Jure Trnovec and Mr. Sebastjan Zorzut, I-Tech, Solkan, Slovenia, 7. 12. 2021

STAFF

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2. Denise Neudecker, Oscar Cabellos, Alexander R. Clark, Wim Haeck, Roberto Capote, Andrej Trkov, Morgan C. White, Michael E. Rising, "Which nuclear data can be validated with LLNL pulsed-sphere experiments?", *Annals of Nuclear Energy*, 2021, **159**, 108345.
3. Luca Fiorito, Pablo Romojaro, Oscar Cabellos, M. García-Hormigos, Augusto Hernandez Solis, S. Sanchez-Fernandez, Alexey Yu Stankovsky, Gert Van den Eynde, Gašper Žerovnik, "On the use of criticality and depletion benchmarks for verification of nuclear data", *Annals of Nuclear Energy*, 2021, **161**, 108415.
4. Mike Herman *et al.* (13 authors), "Infrastructure for the new paradigm of nuclear reaction evaluation", *Annals of Nuclear Energy*, 2021, **163**, 108494.
5. Marco T. Pigni, Roberto Capote, Andrej Trkov, "Progress on the reevaluation and validation of the $n+^{233}$U neutron cross sections ", *Annals of Nuclear Energy*, 2021, **163**, 108595.
6. Vladimir Sobes, Cyrille de Saint-Jean, Dimitri Rochman, Oscar Cabellos, Andrew Holcomb, Eric Bauge, Roberto Capote, Andrej Trkov, Michael Fleming, "WPEC Subgroup 44 computational Inter-comparison exercise on correlations in nuclear data libraries", *Annals of Nuclear Energy*, 2021, **164**, 108605.
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8. Michal Koštál *et al.* (13 authors), "Testing of various neutron filters in reference neutron field in LR-0 reactor for nuclear data validation and verification", *Applied Radiation and Isotopes*, 2021, **169**, 109566.
9. Arran George Plant, Bor Kos, Anže Jazbec, Luka Snoj, Vesna Najdanović-Visak, Malcolm John Joyce, "Nuclear-driven production of renewable fuel additives from waste organics", *Communications chemistry*, 2021, **4**, 132.
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15. Jonathan Naish, Paola Batistoni, Bor Kos, Barbara Obryk, Rosaria Villari, Theodora Vasilopoulou, Ion Stamatelatos, JET Contributors, "Comparison of neutron flux streaming calculations to the 2019-2020 JET experimental deuterium-deuterium results", *Fusion engineering and design*, 2021, **170**, 112538.
16. Igor Lengar, Domen Kotnik, Bor Kos, Aljaž Čufar, Christian Bachmann, Luka Snoj, "Shutdown dose rate calculations with modified DEMO single sector model", *Fusion engineering and design*, 2021, **171**, 112569.
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19. Luka Pirker *et al.* (11 authors), "Sterilization of polypropylene membranes of facepiece respirators by ionizing radiation", *Journal of membrane science*, 2021, **619**, 118756.
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32. Žiga Štancar *et al.* (20 authors) and JET Contributors, "Experimental validation of an integrated modelling approach to neutron emission studies at JET", *Nuclear fusion*, 2021, **61**, 12, 126030.

33. Valerio Mascolino, Alireza Haghighat, Luka Snoj, "Verification and Validation of RAPID Formulations and Algorithms based on Dosimetry Measurements at the JSI TRIGA Mark-II Reactor", *Nuclear science and engineering*, 2021, **195**, 9, 937-953.

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36. Steven R. Meikle *et al.* (32 authors), "Quantitative PET in the 2020s: a roadmap", *Physics in Medicine & Biology*, 2021, **66**, 06rm01.

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Review Article

1. José Coutinho *et al.* (14 authors), "Silicon carbide diodes for neutron detection", *Nuclear instruments and methods in physics research. Section A, Accelerators, spectrometers, detectors and associated equipment*, 2021, **986**, 164793.

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1. Andrej Žohar *et al.* (19 authors) and JET Contributors, "Long term neutron activation in JET DD operation", In: *ANIMMA 2021, 7th International Conference on Advancements in Nuclear Instrumentation Measurement Methods and their Applications, 21-25 June 2021, Prague, Czech Republic*, Proceedings, (EPJ web of conferences **253**), 2021, 03005.

2. Valentin Valero, Licia Ottaviani, Abdallah Lyoussi, H. Ghninou, Vladimir Radulović, Luka Snoj, Anže Pungerčič, A. Volte, M. Carette, C. Reynard-Carette, "3-D thermal and radiation-matter interaction simulations of a SiC solid-state detector for neutron flux measurements in JSI TRIGA Mark II research reactor", In: *ANIMMA 2021, 7th International Conference on Advancements in Nuclear Instrumentation Measurement Methods and their Applications, 21-25 June 2021, Prague, Czech Republic*, Proceedings, (EPJ web of conferences **253**), 2021, 04009.

3. Vladimir Radulović, Loïc Barbot, Grégoire De Izzara, Julijan Peric, Igor Lengar, "Reactor pulse operation for nuclear instrumentation detector testing – preparation of a dedicated experimental campaign at the JSI TRIGA reactor", In: *ANIMMA 2021, 7th International Conference on Advancements in Nuclear Instrumentation Measurement Methods and their Applications, 21-25 June 2021, Prague, Czech Republic*, Proceedings, (EPJ web of conferences **253**), 2021, 04019.

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5. Vladimir Radulović *et al.* (16 authors), "The European nuclear experimental educational platform – ENEEP: Progress, prospects and remote education capabilities", In: *ANIMMA 2021, 7th International Conference on Advancements in Nuclear Instrumentation Measurement Methods and their Applications, 21-25 June 2021, Prague, Czech Republic*, Proceedings, (EPJ web of conferences **253**), 2021, 10002.

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9. Vid Merljak, Marjan Kromar, "Comparing different approaches to calculating decay heat power of a spent fuel dry storage cask for Krško NPP", In: *NENE 2021, 30th International Conference Nuclear Energy for New Europe, September 6-9, Bled, Slovenia*, Proceedings, Nuclear Society of Slovenia, 2021, 304.

10. Daniel Lopéz Aldama, Andrej Trkov, Roberto Capote Noy, "On the processing of thermal scattering law data into ACE format for Monte Carlo transport calculations", In: *NENE 2021, 30th International Conference Nuclear Energy for New Europe, September 6-9, Bled, Slovenia*, Proceedings, Nuclear Society of Slovenia, 2021, 305.

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19. Dušan Ćalić, Marjan Kromar, "Impact of the various nuclear data libraries on the NPP Krško spent fuel characterization", In: *NENE 2021, 30th International Conference Nuclear Energy for New Europe, September 6-9, Bled, Slovenia*, Proceedings, Nuclear Society of Slovenia, 2021, 319.

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Independent Component Part or a Chapter in a Monograph

1. Damijan Valentinuzzi, Katja Uršič Valentinuzzi, Matea Maruna, Simon Buček, Urban Simončič, Martina Vrankar, Maja Čemažar, Gregor Serša, Robert Jeraj, "Computational modeling and experimental investigations to enhance the successful response of anti-PD-1 cancer immunotherapies", In: *The physics of cancer: research advances*, World Scientific, 2021, 145-164.

Theses and Mentoring

1. Jošt Stergar, *Combined hyperspectral imaging of macroscopic and microscopic samples for tissue optical and structural properties evaluation:* doctoral dissertation, Ljubljana, 2021 (mentor Matija Milanič).

DEPARTMENT OF EXPERIMENTAL PARTICLE PHYSICS F-9

Departmental research is devoted to experimental studies of elementary particles, to reveal the ultimate building blocks of matter and the nature of the interactions between them. Experiments are carried out within large collaborative programmes at international centres for particle physics at CERN near Geneva and at KEK in Tsukuba. The department is also engaged in developing and applying technologically advanced particle detectors, which 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.

Head:
Prof. Marko Mikuž

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, an example is the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN) near Geneva. Researchers exploit this facility to perform experiments in presently inaccessible regions of energy, which, though pushed higher and higher, still remain minute compared to that of the vast blast of the Big Bang that led to the creation of the Universe.

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

- ATLAS at the Large Hadron Collider (LHC) at CERN (3000 researchers, 183 institutions from 38 countries),
- Belle II at the asymmetric electron-positron collider (KEK-B) at KEK (1679 researchers, 123 institutions from 26 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 the 2021 activities follows, focused on the contributions of our researchers:

ATLAS experiment

In the past 3 years an upgrade is taking place at CERN, because the Large Hadron Collider (LHC), as well as its detectors, are being upgraded before the next re-start, which gives us much-needed time to analyse the data collected so far. This year the new data taking period, named "Run 3", is starting. The years 2015-2018 mark at CERN the data-taking period of the Large Hadron Collider (LHC) named "Run 2". In the year 2015 the upgraded Large Hadron Collider LHC began its operation at CERN and reached a record centre-of-mass energy of 13 TeV. The end of the "Run 2" of the LHC's operation subsequently finished at the end of 2018 with heavy ion collisions (Pb-Pb) at a centre-of-mass energy of 5.02 TeV. The amount of the ATLAS experiment proton-proton collision data at 13 TeV in the year 2015-2018 reached the integrated luminosity of 150 fb⁻¹ of exceptional data, whereby the LHC exceeded all expectations and facilitated the recording of the largest quantity of data at the ATLAS experiment so far. This set of unique data (Figure 1) led to the most precise Run 2 searches for new physics beyond the Standard Model hitherto achieved. In the analyzed data new limits on dark matter searches were set as well as the first results of a spectral correlation analysis of heavy ion

In the analysed data, new limits on dark-matter searches were set as well as the first results of spectral correlation analysis of heavy ion collisions (Xe + Xe)
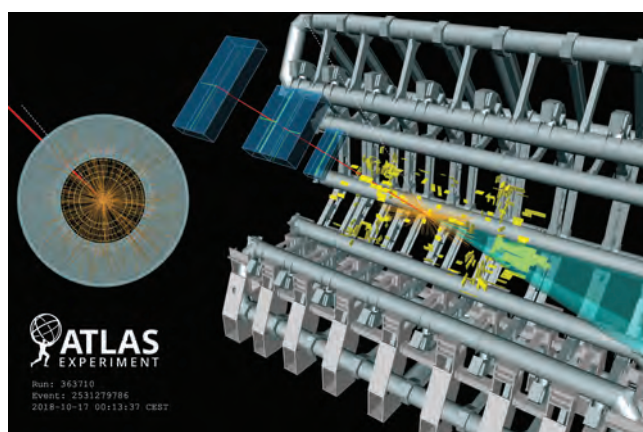
Figure 1: Event display associated to search for heavy resonances decaying into a W boson and a Higgs boson in final states with leptons and b-jets in pp collisions at 13 TeV with the ATLAS detector. The W boson candidate is comprised of the muon and missing transverse energy, where the muon is indicated by the red line and the missing transverse energy is indicated by the dotted white line. The Higgs boson candidate is comprised of the large jet, indicated by the blue cone. The yellow blocks correspond to energy depositions in the hadronic calorimeter.
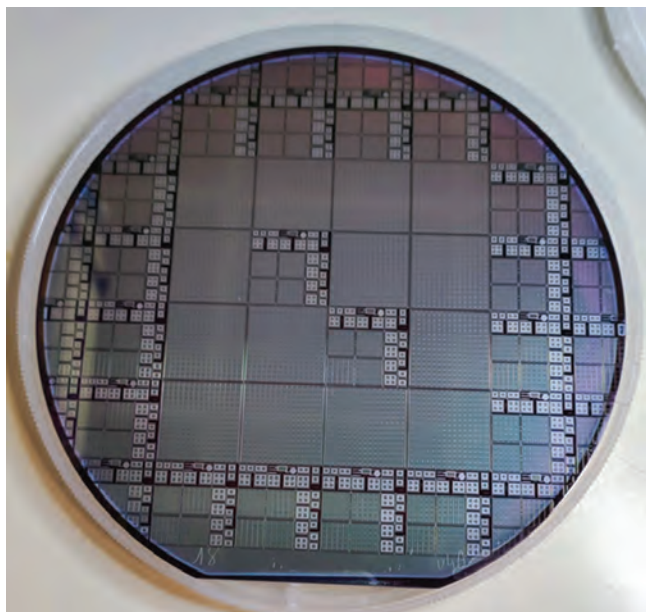
Figure 2: A photo of a 6" silicon wafer with large multi-channel LGAD (15×15 pads) produced at FBK which are suitable for the ATLAS experiment. These sensors use a carbon-enriched gain layer.

collisions (Xe + Xe); furthermore, rare Higgs boson decays were detected for the first time ($H \to \mu\mu, H \to Z\gamma$), for a final confirmation of these measurements, however, more data is needed. In addition, a considerable number of different theories, which extend the Standard Model, were excluded and there are some indications for potential new discoveries in particle physics. However, for confirming or refuting these the full set of recorded data needs to be analysed. The next year will still be full of challenges and expectations of pivotal events. In 2021 the ATLAS collaboration published more than 60 scientific papers in the most distinguished scientific journals, bringing the total number of scientific papers published by the collaboration to 1030, with more than a hundred further papers in preparation.

ATLAS Ljubljana group plays the leading role in designing, building and operating several beam- and radiation-monitoring systems: ATLAS Beam Condition Monitor (BCM), Beam Loss Monitor (BLM), Radiation Monitor (RADMON) and Diamond Beam Monitor (DBM). BCM was built to monitor conditions of the LHC beams and issue warnings about unexpected and potentially dangerous situations. In the first part of the LHC's operation it served as the main luminosity monitor of ATLAS. BLM, on the other hand, is solely a safety system and protects ATLAS Inner Detector from potential damage by LHC beams. BLM operates independently in parallel with BCM. It fired a few times and successfully extracted LHC beams and prevented potential damage to the detectors. RADMON records the doses received by different parts of the ATLAS Inner Detector. In 2021 readout electronics and control software of the BCM was upgraded and, together with BLM, re-integrated into the ATLAS data-acquisition system and prepared for taking data in 2022.

Atlas detector upgrade

In 2021 the LHC was preparing for the new data-taking period "Run 3" which will start in 2022 and will go on until the end of 2025. After "Run 3" a major upgrade of the LHC to the High Luminosity LHC (HL-LHC) will start. The beginning of the HL-LHC's operation is scheduled for 2028. To adapt to HL-LHC conditions a major upgrade of the ATLAS detector will be made during this shutdown period. A large part of the ATLAS collaboration, including the group from the F9 department, is intensively working on the development and the building of detector systems for the upgrade.

The operation of LGADs in High Granularity Timing Detector in ATLAS will be limited to much lower bias voltages than in the laboratory because of destructive events – single-event burnout. This effect will make the use of carbon-enriched sensors mandatory in ATLAS.

The group from the F9 department has taken the leading role in the development of a new system, based on pCVD diamond sensors, named BCM'. It will replace the current beam abort and luminosity monitors. A dedicated rad-hard ASIC readout chip Calypso, which will be used to amplify and discriminate the signals coming from the segmented pCVD diamond sensor, has been developed. In 2021 the radiation hardness of the chip was verified in several irradiation experiments. The performance of the diamond sensor read out by the new chip was successfully tested in the test beam. Various components of the system were designed and manufactured, and their functionality verified. BCM' is placed near the interaction point and is a subsystem of the pixel detector. Support structure and electrical and data connections must be harmonized with that of the pixel detector system and comply with very strict engineering and radiation-hardness constraints.

The High Granularity Timing Detector has officially become part of an ATLAS upgrade for the High-Luminosity LHC upgrade in 2020. The JSI group has taken a large part in the development and testing of suitable Low Gain Avalanche Detectors (LGADs) for the HGTD (Figure 2) as documented in several publications. We tested sensors from different producers and showed their suitability for use in the ATLAS experiment. The dependence of charge collection and timing properties of the sensors on neutron fluence were systematically measured. We contributed to the development of different LGAD gain layer designs and showed the beneficial effect of carbon co-implantation on the radiation hardness of the LGADs, particularly the reduced acceptor removal. Measurements in the beam of highly energetic particles showed
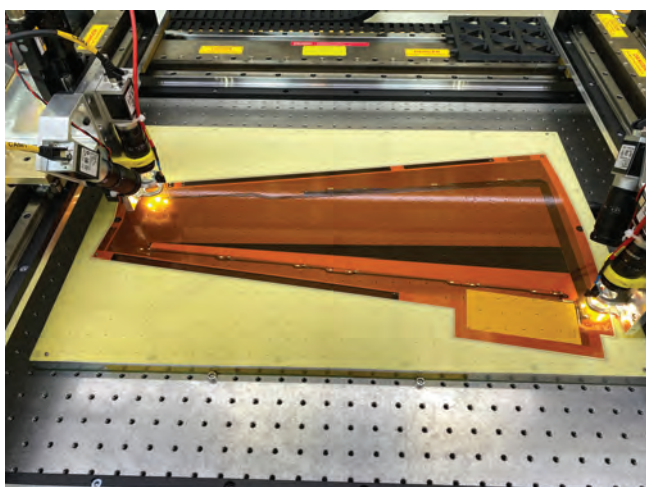

Figure 3: The photograph shows the robot testing a flexible circuit. Two movable test stations equipped with cameras can be seen. Stations electrically contact the circuit and measure its properties and detect irregularities.

that the use of LGADs is limited to much lower voltages than in the laboratory, due to destructive events (single event burnout), which make the use of carbon-enriched sensors mandatory in ATLAS. We demonstrated the stable operation of large LGAD arrays, irradiated and non-irradiated, over prolonged periods of time in similar conditions, as expected in the ATLAS experiment.

In 2021 the ATLAS collaboration continued assembling components to upgrade the inner part of the detector (Inner tracker – ITk). Silicon microstrip sensors will be used for tracking charged particles. By the end of 2021 ATLAS assembled about 5% of the components, which represents pre-series production. Our group participates in the process of ensuring the quality of the sensors (QA). At the reactor centre in Podgorica we irradiated test structures made on silicon wafers with neutrons. Regular irradiations are planned every month for a period of 4 years. In a specially designed measurement setup, we measure the response of the sensors to electrons from a ^{90}Sr source with the ALIBAVA multi-channel readout system. All the sensors from the pre-series showed the expected degradation of the signals, the signal is reduced to about a third after irradiation with $1.6 \cdot 10^{15}$ n_{eq} cm^{-2}, this corresponds to about 7500 electrons. Measurements on pre-series sensors showed the expected results, in the second half of 2021 we began with an evaluation of sensors produced in serial production.

More than 1000 large flexible circuits for silicon strip detector modules will be produced. Each circuit will be tested three times in different stages of detector assembly process.

In addition to sensors' development we took part in the development of special multilayer flexible circuits together with the company Elgoline d.o.o. These radiation hard circuits connect sensors with peripheral read-out electronics. The preproduction (5% of the whole production) was completed in 2021. Together with Oxford University a robot for testing these circuits was developed (Figure 3). Elgoline will produce more than 1000 of such large flexible circuits in 2021/2022 for the assembly of two endcaps of ITk. Each circuit will be tested three times at different stages of the assembly process.

An upgraded system for online measurements of integrated doses (RadMon) will be installed in the ITk. In 2021 our group designed and manufactured the first prototypes of a radiation sensor module hosting RadFETs and diodes. The response of the sensor to the radiation was tested in the reactor in Podgorica. A prototype of readout system was designed and the first components have been built.

Belle detector at the asymmetric electron positron collider KEKB at K

Collaborators at the department continued activities at the Belle and Belle II experiments at the electron positron collider KEKB (SuperKEKB) in Tsukuba, Japan. The main motivation for the two experiments, belonging to the so-called Intensity Frontier Experiments, is searching for so-far-unknown processes and particles beyond the theory of the Standard Model (SM) and is commonly addressed as the New Physics (NP). Intensity Frontier Experiments perform measurements of ultra-high precision to compare the results to equally precise predictions of the SM. The latter is nowadays considered as the most successful and experimentally verified theory of elementary particles' interactions at the currently achievable energies and precision. NP processes must be responsible – among other aspects – for the observed dominance of matter over anti-matter in the Universe.

While the Belle experiment finished data-taking in 2010, numerous analyses of the data are still in progress. Among the results published in 2021 are the first measurements of differential branching fractions of inclusive semi-leptonic $B \rightarrow X_u l^+ \nu_l$ decays. The measured distributions are sensitive to the shape function governing the nonperturbative dynamics of the $b \rightarrow u$ transition and provide the necessary experimental input for future model-independent approaches of the determination of the CKM matrix element $|V_{ub}|$. These measurements will hopefully help to resolve the persistent tension observed in the value of $|V_{ub}|$ as determined from exclusive and inclusive studies.

Figure 4: Measured value of $R_{K^*} = Br(B \rightarrow K^* e^+ e) / Br(B \rightarrow K^* \mu^+ \mu)$ as a function square of lepton pair momentum (q^2) along with the SM prediction. Results are consistent with expectations; however, the shift in the first bin towards lower value points in the same direction as LHCb observed anomaly.

Another high-impact result of the Belle collaboration in 2021 was a new test of lepton-flavour universality through the measurement of $B \rightarrow K^* l^+ l^-$. Due to several anomalies observed in recent years in the B decays mediated by the $b \rightarrow s\, l^+ l^-$ transition (mainly by the LHCb experiment), this measurement is of great interest to the community. For the first time, this measurement included decays with K^{*+} in the final state in addition to K^{*0}. The result (Figure 4) is consistent with the SM prediction as well as with the LHCb results. Larger data sets, which will be provided in the next years by the Belle II and LHCb experiments, are needed to resolve the presently observed anomalies.

The Belle II experiment has so far collected 270 fb^{-1} of data, with the SuperKEKB breaking the instantaneous luminosity world record several times in 2021. Among the important results of the Belle II collaboration in 2021

Figure 5: Decay-time distributions of (top) $D^0 \rightarrow K^- \pi^+$ and (bottom) $D^+ \rightarrow K^- \pi^+ \pi^+$.

is the world's most precise measurement of D^0 and D^+ lifetimes (figure 5). This measurement demonstrates the excellent vertexing capabilities of the Belle II detector and confirms a good understanding of systematic effects that will impact future analyses of neutral-meson mixing and mixing-induced CP-violation. Another prominent result comes from the search for the $B^+ \rightarrow K^+ \nu\nu$ decay [4]. Within the SM this decay is too rare to be observed with the present amount of data, but in several NP models its branching fraction is enhanced. Because the measurable decay signature involves only a single charged kaon, a novel experimental approach is used that exploits not only the properties of the $B^+ \rightarrow K^+ \nu\nu$, but also the inclusive properties of the other B meson in the $Y(4S) \rightarrow B\bar{B}$ event (so-called inclusive tagging). In this study, no significant signal is observed, and an upper limit on the branching fraction is set. Despite the small data sample used for the measurement (~70 fb^{-1}) the limit is competitive with other measurements. This demonstrates the capability of the inclusive tagging approach, which is widely applicable, and will expand the future physics reach of the Belle II experiment.

Pierre Auger observatory

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

The world's most precise measurement of the D meson lifetime and the measurement of the $B^+ \rightarrow K^+ \nu\nu$ branching fraction at the Belle II experiment are pointing towards numerous new results that will follow in the upcoming years from this experiment.

The Pierre Auger Observatory combines two complementary techniques to measure the air showers. On their way through the atmosphere the secondary particles stimulate nitrogen molecules in the air to emit fluorescent light. This light is measured with large telescopes. In addition, secondary particles reaching ground level are registered in an array of particle detectors. The latter are water Cherenkov detectors, measuring the light emitted by relativistic particles passing through a water tank.
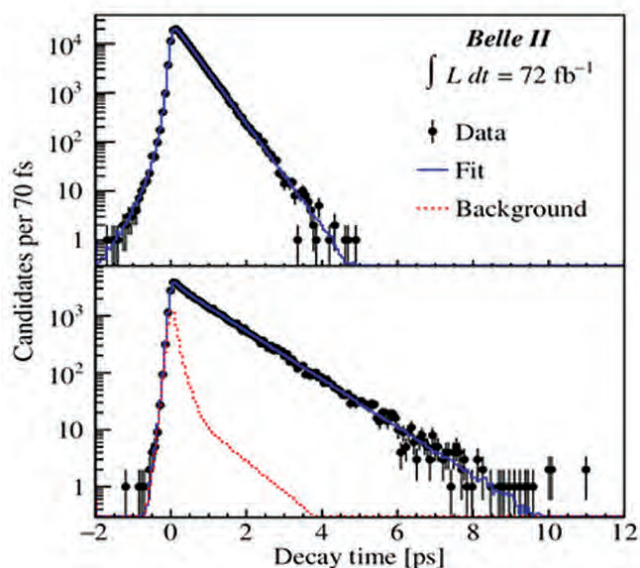
The Pierre Auger Collaboration had shown that the energy spectrum of cosmic rays exhibits a sharp drop around 10^{20} eV. This drop is compatible with the Greisen-Zatsepin-Kuzmin (GZK) cut-off caused by the universe becoming opaque due to resonant collisions between ultra-high-energy protons and the photons of the cosmic microwave 2.7-K background radiation. Past measurements by the Pierre Auger Collaboration have already cast some doubt on this explanation, and this year's results further established that the GZK cut-off cannot be the entire story and even the extent of its contribution to the cut-off remains unclear.

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

The Pierre Auger observatory is currently upgrading its detection capabilities. The key element of the upgrade is the installation of a plastic scintillator on top of each existing surface detector station. It will provide a complementary measurement of the showers, allowing the reconstruction of muons and electromagnetic particles. The surface scintillator detector stations (SSDs) are being deployed over the full 3,000-km^2 area of the overall surface detector (SD). To enhance the capabilities of the surface detector,

Figure 6: The equipment of SiGNET computing centre is at Teslova 30 (photo) and Jamova cesta 39 in Ljubljana. The centre is connected to Academic and research network of Slovenia (ARNES) with a 100 Gb/s link.

especially for composition measurements, it is being equipped with upgraded electronics that have a larger sampling rate and a larger dynamic range.

Commissioning of the AERA system (Auger Engineering Radio Array) is also under way. AERA is a new antenna system to measure short radio pulses emitted by cosmic-ray air showers of the highest energies. It consists of an array of antennas sensitive in the frequency range of 30 to 80 MHz with signal processing and electronics developed specifically for this purpose.

Distributed computing

In 2021 the SiGNET Tier-2 computing centre, with over 7000 cores and around 5 PB of storage capacity (Figure 6), continued its collaboration on international projects and the organisations WLCG, EGI, EGI/InSPIRE, Nordugrid. Furthermore, we worked together with other computing centres such as the Institute's own NSC and Arnes centre. As a part of the European initiative EuroHPC and the Slovenian national supercomputing network SLING, we participated in the setting up and maintenance of the Vega supercomputer at IZUM in Maribor. The resources of the SiGNET centre were, in 2021, used mainly for the data analysis of international experiments ATLAS and Belle II, as well as for other department's projects. Some of the resources were also available for other Institute departments and for external collaborators. We have also continued with cooperation in the Leonardo project, in setting up one of the three pre-exascale HPC systems in Cineca, Bologna. Apart from maintenance and administration, the department also collaborates in numerous projects related to the support, maintenance and planning of the computing infrastructure as well as to the development, distribution and deployment of the distributed computing infrastructure.

In 2021 we participated in setting up and maintenance of the Vega supercomputer at IZUM in Maribor.

Detector development
Silicon and diamond detectors

Most of the work on silicon detector development was performed in the framework of the ATLAS and CERN-RD50 collaborations. Our group is also active in the development of diamond tracking detectors within the RD42 collaboration.

Work on an upgrade of the ATLAS detector for the HL-LHC was the main activity related to the development of silicon detectors. This includes measurements of silicon strip detectors and the development of LGAD for HGTD, as described above. In addition to work for ATLAS' extensive measurements with depleted CMOS detectors were made in 2021. Depleted CMOS is a suitable technology for monolithic tracking detectors for high radiation environments as well as for applications where the amount of material in the tracking volume must be minimized. Depleted CMOS ensures also fast charge collection enabling good time resolution, which is becoming increasingly important in all types of applications. In 2021 we measured the time properties of active pixels in an RD50-MPW2 chip. First we made a study of the position-dependent timing response using E-TCT. The study showed that the timing properties of the amplifier significantly affect detector efficiency.

For the development of the innovative fluorescence lifetime measurement method, we received the award for the best innovative project at the International Technology Transfer Conference.

Our group is active in detector development for next-generation hadron colliders such as Future Circular Collider - FCC_{hh}. Work includes measurements of the detector response after irradiation to extreme hadron fluences of 10^{17} n/cm^2 and beyond. In 2021 several measurements with detectors irradiated to extreme fluence were made.

The work with diamond detectors was, in 2021, focused on the development of sensors for BCM'. Measurements in the test beam were made with 1 cm × 1 cm, 500-μm-thick, diamond sensor. The diamond surface was covered with collection electrodes with several sizes. They were connected to the Calypso readout chip, which is an ASIC developed for BCM'.

In the framework of a bilateral project with the NürDAM institute, Bolu, Turkey, FET dosimeters with different dielectrics were investigated with the aim of increasing their sensitivity. MOSFET structures with a thin layer of HfO_2 replacing SiO_2 were manufactured and their response to radiation tested. It turned out that the charge accumulation in HfO_2 is slower than in SiO_2, which means a lower sensitivity of HfO_2 devices.

Figure 7: Prototype of a Ring Imaging Cherenkov (RICH) detector with an aerogel radiator. Left: Cherenkov photons emitted by charged particles in an aerogel layer are detected by a matrix of photosensors, capable of detecting single photons. Right: reconstructed hits of single photons on the detector plane.

Photon detectors

In 2020, we continued with the research of photon sensors for the new generation of Cherenkov ring detectors (RICH). For the upgrade of the Belle II detector in the forward direction and the upgrade of the Cherenkov ring detectors of the LHCb spectrometer, we are developing a single photon sensor that will be very fast, will have fine granulation, will be sensitive to light of

long wavelengths and withstand radiation load, mainly due to neutron flux. We studied various detector candidates and radiators. In the high-energy charged particle test beam at CERN (Figure 7), we tested prototype detectors equipped with silicon photomultipliers, photomultipliers with microchannel plates and the latest aerogel samples with different refractive indices

Detectors for medical applications

Experimental particle physics strives to develop and master state-of-the-art technology. Innovations from our laboratories can be usefully transferred to other areas. Medical physics is a successful example where we are introducing advances in photodetectors and reading electronics to improve detector technology in nuclear medicine and imaging methods in biomedical optics.

Based on our in-depth understanding of detector response and data analysis methods we contributed to the development and evaluation of the performance of novel biomarkers for PET used in cancer studies and for the prediction of COVID-19 disease severity.

Figure 8: The use of ultra-fast detectors enables affordable positron tomography of the entire human body with the same image quality as current commercial state-of-the-art. The figure shows the results of simulations with flat-panel detectors covering almost the entire human body.

We have designed a positron-emission tomography (PET) device with flat-panel detectors, which, based on ultra-fast detection, enables PET imaging with a significantly smaller amount of detection crystal, thus enabling a lower cost and greater flexibility. Through precise simulations, we have shown that such an approach achieves image quality comparable to the best current commercial devices, while also enabling more affordable simultaneous imaging of the whole body (Figure 8). We are involved in an international cooperation to develop such a PET device, which includes the University of Barcelona, Fondazione Bruno Kessler, University of Davies in California and Harvard University.

We have developed a system for fluorescence lifetime measurements that uses the latest light detectors to enable faster acquisition than existing methods. For the development of the innovative fluorescence lifetime measurement method, we have received the Best innovative projects within public research organizations for the economy in 2021 prize, at the 14th International Technology Transfer Conference 2021 organized by the Jožef Stefan Institute Centre for Technology Transfer and Innovation. With experience in advanced light-detection methods, we also participated in the construction and first preclinical measurements with a hyperspectral imaging system.

Based on our in-depth understanding of detector-response and data-analysis methods, we also contributed to the development and evaluation of the performance of novel biomarkers for PET, used in cancer studies and the prediction of COVID-19 disease severity.

Irradiations in reactor TRIGA

A significant number of irradiations with neutrons, as well as with ionizing radiation of the reactor core when fission is stopped, was made for various institutions from around the world. Reactor at IJS is the reference neutron irradiation site for development of silicon detectors and electronics for LHC and other particle-physics experiments.

ERC project

1. H2020 - FAIME; Flavour Anomalies with advanced particle Identification Methods
Prof. Peter Križan
European Commission

Some outstanding publications in the past year

[1] G. Aad et al (ATLAS Collaboration), "*Search for Dark Matter produced in association with a dark Higgs boson decaying into $W^\pm W^\mp$ or ZZ in fully hadronic final states from $\sqrt{s}$=13 TeV pp collisions recorded with the ATLAS detector*". Phys. Rev. Lett., 126, 121802, (2021).

[2] G. Aad et al (ATLAS Collaboration), "*Longitudinal flow decorrelations in Xe+Xe Collisions at $\sqrt{s_{NN}}$=5.44 TeV with the ATLAS Detector*". Phys. Rev. Lett., 126, 122301 (2021).

[3] G. Aad et al (ATLAS Collaboration), "*Search for lepton-flavor violation in Z-boson decays with τ leptons with the ATLAS detector*", Phys. Rev. Lett, 127, 271801, (2021).

[4] G. Aad et al (ATLAS Collaboration), "*Search for displaced leptons in $\sqrt{s}$=13 TeV pp collisions with the ATLAS detector*", Phys. Rev. Lett., 127, 051802 (2021).

[5]   G. Aad et al (ATLAS Collaboration), *"Test of the universality of τ and µ lepton couplings in W-boson decays with the ATLAS detector".* Nature physics, 2021, vol. 17, no. 7, str. 813-818.

[6]   L. Cao *et al.* (Belle Collaboration), *"Measurement of Differential Branching Fractions of Inclusive $B{\to}X_u l^+ \nu_l$ Decays"*, Phys. Rev. Lett. 127, 261801 (2021).

[7]   S. Wehle *et al.* (Belle Collaboration), *"Test of Lepton-Flavor Universality in $B{\to}K^* l^+ l^-$ Decays at Belle"*, Phys. Rev. Lett. 126, 161801 (2021).

[8]   F. Abudinén *et al.* (Belle II Collaboration), *"Precise Measurement of the D^0 and D^+ Lifetimes at Belle II"*, Phys. Rev. Lett. 127, 211801 (2021).

[9]   F. Abudinén *et al.* (Belle II Collaboration), *"Search for $B^+{\to}K^+\nu\nu$ Decays Using an Inclusive Tagging Method at Belle II"*, Phys. Rev. Lett. 127, 181802 (2021).

[10] A. Aab et al. (Pierre Auger Collaboration), *"Measurement of the Fluctuations in the Number of Muons in Extensive Air Showers with the Pierre Auger Observatory"*, Phys. Rev. Lett. 126, 152002 (2021).

Awards and Appointments

1.   Dr Andrej Seljak, Dr Rok Dolenec, Dr Rok Pestotnik, Prof. Peter Križan, Prof. Samo Korpar: Best innovative projects within public research organizations for the economy in 2021 prize Title: Real-time fluorescence lifetime acquisition system – RfLAS, Center for Technology Transfer and Innovation, Jožef Stefan Institute, Ljubljana, Slovenia

Organization of Conferences, Congresses and Meetings

1.   Researchers' Night, Jožef Stefan Institute, Ljubljana, Slovenia, 24 September 2021

INTERNATIONAL PROJECTS

1.   **ERC H2020 - FAIME; Flavour Anomalies with advanced particle Identification Methods**
     Prof. Peter Križan
     European Commission
2.   COST CA16108 - VBSCan; Vector Boson Scattering Coordination and Action Framework
     Prof. Borut Paul Kerševan
     Cost Office
3.   COST VBSCan; Vector Boson Scattering Coordination and Action Framework
     Prof. Borut Paul Kerševan
     Cost Association Aisbl
4.   H2020 - JENNIFER2; Japan and Europe Network for Neutrino and Intensity Frontier Experimental Research 2
     Prof. Rok Pestotnik
     European Commission
5.   H2020 - EUROCC; National Competence Centres in the Framework of EuroHPC
     Prof. Marko Mikuž
     European Commission
6.   H2020 - AIDAinnova; Advancement and Innovation for Detectors at Accelerators
     Dr. Gregor Kramberger
     European Commission
7.   H2020 - HITRIplus; Heavy Ion Therapy Research Integration
     Asst. Prof. Andrej Studen
     European Commission
8.   Fabrication and Qualification of NürFETs Dosimeters for use at Nuclear Reactors
     Dr. Gregor Kramberger
     Slovenian Research Agency
9.   Development of Segmented Silicon and Diamond Radiation Sensors and Readout Electronics for Particle Physics and Medical Diagnostics
     Asst. Prof. Igor Mandić
     Slovenian Research Agency
10. Study of Portion and Spatial Resolution of High-Resolution Events on Image Quality in Hybrid Resolution PET Systems
     Prof. Vladimir Cindro
     Slovenian Research Agency

RESEARCH PROGRAMMES

1.   Astroparticle Physics
     Prof. Marko Zavrtanik
2.   Experimental Particle Physics
     Prof. Borut Paul Kerševan

R & D GRANTS AND CONTRACTS

1.   New atmospheric monitoring devices and techniques for Imaging Atmospheric Cherenkov Telescopes
     Prof. Marko Zavrtanik
2.   Advanced detector for Time-of-Flight PET based on Cherenkov radiation
     Prof. Samo Korpar
3.   Application of Machine Learning Methods in the Data Analysis at the Large Hadron Collider (LHC)
     Dr. Andrej Gorišek
4.   Atmospheric remote sensing for Cherenkov Telescope Array and its impact on science from large sky survey observations
     Prof. Marko Zavrtanik
5.   Depleted CMOS Sensors for the ATLAS Tracker Upgrade and Future Collider Experiments
     Prof. Marko Mikuž
6.   Advanced hadron identification methods for Belle II
     Prof. Peter Križan
7.   Development of High Granularity Timing Detector for ATLAS experiment
     Dr. Gregor Kramberger
8.   ITk - Upgrade of the ATLAS Tracker for High-Luminosity LHC
     Prof. Marko Mikuž
9.   Collaboration CERN RD-39
     Prof. Marko Mikuž
     Cern
10. Collaboration CERN RD-50
     Prof. Marko Mikuž
     Cern
11. Collaboration DELPHI
     Prof. Borut Paul Kerševan
     Cern
12. Collaboration ATLAS
     Prof. Marko Mikuž
     Cern
13. Collaboration CERN RD-42
     Prof. Marko Mikuž
     Cern
14. Collaborations Belle in Belle II
     Prof. Peter Križan
     Kek - High Energy Accelerator Research
15. Design, Procurement and QA of Flex-rigid Hybrids
     Prof. Marko Mikuž
     European Organization For Nuclear Research
16. Irradiations in TRIGA Nuclear Reactor
     Prof. Vladimir Cindro

VISITORS FROM ABROAD

1.   Dr Karol Adamczyk, Henryk Niewodniczański Institute of Nuclear Physics, Krakov, Poland, 31 August – 1 September 2021
2.   Dr Rafaelle Giordano, University of Naples Federico II, Naples, Italy, 19 September – 25 September 2021
3.   Andrea Crnjac, Dr Miloš Manojlović, Ruđer Bošković Institut, Zagreb, Croatia, 14 December – 16 December 2021

STAFF

Researchers
1. Dr. Karol Mateusz Adamczyk
2. Asst. Prof. Marko Bračko*
3. Prof. Vladimir Cindro
4. Prof. Andrej Filipčič
5. Prof. Boštjan Golob*
6. Dr. Andrej Gorišek
7. Prof. Borut Paul Kerševan*
8. Prof. Samo Korpar*
9. Dr. Gregor Kramberger
10. Prof. Peter Križan*
11. Dr. Boštjan Maček
12. Asst. Prof. Igor Mandić
13. **Prof. Marko Mikuž*, Head**
14. Prof. Rok Pestotnik
15. Asst. Prof. Tomaž Podobnik*
16. Dr. Andrej Seljak
17. Prof. Marko Starič
18. Asst. Prof. Andrej Studen*
19. Prof. Marko Zavrtanik
20. Prof. Danilo Zavrtanik*
21. Asst. Prof. Dejan Žontar*

Postdoctoral associates
22. Dr. Rok Dolenec*

23. Dr. Bojan Hiti
24. Dr. Luka Šantelj

Postgraduates
25. Dania Consuegra Rodriguez, M. Sc.
26. Alissa Shirley-Ann Howard, M. Sc.
27. Blaž Leban, B. Sc.
28. Andrej Lozar, B. Sc.
29. Miha Mali, B. Sc.
30. Jakob Novak, B. Sc.
31. Anja Novosel, B. Sc.
32. Leonardo Benjamin Rizzuto
33. Luka Senekovič, B. Sc.

Technical officer
34. Jakob Merljak, B. Sc.

Technical and administrative staff
35. Andreja Butina Čalič, B. Sc.
36. Jurij Eržen
37. Dejan Lesjak
38. Erik Margan

Note:
* part-time JSI member

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DEPARTMENT OF INORGANIC CHEMISTRY AND TECHNOLOGY K-1

The Department of Inorganic Chemistry and Technology is one of the world's leading groups for the synthesis of new inorganic compounds containing fluorine. The main research areas are: the synthesis of new coordination compounds with various ligands, the chemistry of noble gases, the chemistry of the main-group elements, the synthesis of new hybrid materials and inorganic materials with special properties. A large part of the group's activities is devoted to technological, environmental and process safety issues in Slovenia. The group has been working closely with Slovenian industry for more than thirty years. It is also active in the field of education and the promotion of science.

Head:
Asst. Prof. Gašper Tavčar

In 2021 we renovated the laboratory space and equipped the Extreme Conditions Chemistry Laboratory, which is being built by the researchers from departments K1 and K5, the winners of the Director's Fund project. The installed equipment includes a system of two gloveboxes with a built-in stereomicroscope and ATR-FTIR spectrometer, as well as a new state-of-the-art Rigaku Oxford Diffraction XtaLAB Synergy-S single-crystal X-ray diffractometer funded by the ERC StG project. This instrument is equipped with a modern Dectris Eiger2 R CdTe detector and a short-wavelength silver microfocus tube in addition to a copper microfocus X-ray tube, making it particularly suitable for crystal structure determinations at high pressure in diamond-anvil cells. This will be used in the HiPeR-F project, focused on the study of chemical reactions with fluorine under extremely high pressure – from 10,000 bar to over 100,000 bar. The fluorine element, which can be called the tiger of the periodic table due to its extraordinary reactivity, will make it possible to test the limits of chemistry under extreme conditions. This research is thus a combination of two specialized experimental as well as extreme research areas – the study of substances under extremely high pressures and the study of extreme chemical reactivity.

Chemical properties of substances can also be investigated under extreme conditions in a renovated laboratory equipped with modern equipment.

Research in coordination chemistry was carried out with different ligands. Noble-gas chemistry continues to be an important part of the research activities. Removal of volatiles at 243 K from solutions of LnF_3 (Ln = La - Dy and Y) and XeF_2 (molar ratio 1:3) in anhydrous HF acidified with an excess of BF_3 gave $[Ln(XeF_2)_3](BF_4)_3$ salts. Reactions carried out in the same way but with a molar ratio of $LnF_3 : XeF_2 = 1:1$ gave $[Ln(XeF_2)](BF_4)_3$ salts (La - Nd). The crystal structures of the La and Nd salts are isotypic. Using a molar ratio of $LnF_3 : XeF_2 = 1:2$ and the same synthetic approach, only the La-compound was prepared as the $[La(XeF_2)_2](BF_4)_3$ salt. Prolonged pumping of $[Ln(XeF_2)_n](BF_4)_3$ (n = 3, 2, 1) at 298 K or experiments with isolation at 298 K led to products with a lower XeF_2 content or to mixtures of different products. In addition to the $[Ln(XeF_2)](BF_4)_3$ and LnF_3/BF_3 products, the $[Ln(XeF_2)]F(BF_4)_2$ salts (Ln = La, Nd, Sm, Eu, Tb, Dy and Y) were also formed. The crystal structures of $LaF(HF)(BF_4)_2$ and $LaF(BF_4)_2$ by-products were determined.

Coordination chemistry connected with imidazolium compounds including N-heterocyclic carbenes resulted in the synthesis, characterization and detailed analysis of the bonds using DFT calculations of compounds $[(LDipp)H][VOF_4(THF)]$ and $[(LDipp)H][VOF_4(Py)]$. We focused on studying the nature of bonding between the VOF_4^- anion and various ligands such as THF, pyridine (Py), ABCO, methane, ethylene, water, acetonitrile and ammonia. The nature of the bonds between the units in the compounds is often inferred from single-crystal analysis data. With the DFT calculations, we can study the interactions in more detail and get a different view of individual interactions between the units. With this study, we have shown that relying solely on the structural aspects of solved crystal structures, such as ligand orientation and bond distances, can lead to a misinterpretation of the chemical bonds. The research was carried out in collaboration with the Department of Physical and Organic Chemistry of the Jožef Stefan Institute. Furthermore, we studied N-heterocyclic carbenes coordinated to alane, where we introduced a new method for the selective functionalization of alanes. Aldiminium-based triflate or chloride salts were used as the group transfer reagent for Cl^- and $CF_3SO_3^-$ units. This reaction proceeds quantitatively in a 1:1 molar ratio resulting in the isolation of $[(IPr)AlH_2OTf]$, $[(IPr)AlH_2Cl]$ and $[(IPr)AlHCl_2]$ compounds, which were also structurally characterized.
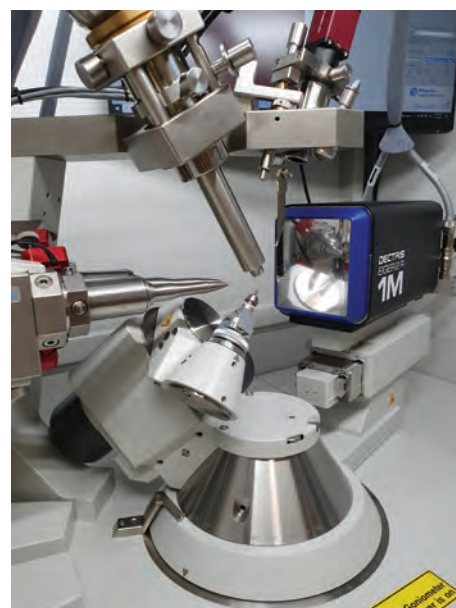

Figure 1: Modern state-of-the-art single-crystal X-ray diffractometer Rigaku OD XtaLAB Synergy-S

Figure 2: Glovebox system in the Extreme Conditions Chemistry Laboratory

We need a comprehensive and critical view of the effects of fluoride ions and organofluorine compounds on human health and the environment.
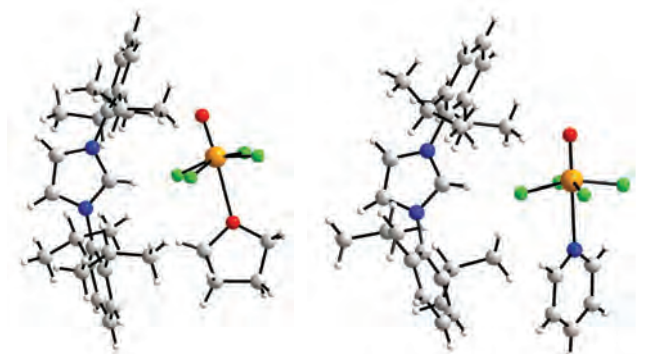
Figure 3: Crystal structures of $[(L^{Dipp})H][VOF_4(THF)]$ (a) and $[(L^{Dipp})H][VOF_4(Py)]$ (b), published in Inorganic Chemistry, 2021, 60, 11932–11947

Figure 4: Effects of fluoride ions and organofluorine compounds on human health and environment, published in Chemical Reviews, 2021, 121, 4678–4742

The studies included ambisaline ions of nitrogen, oxygen and fluorine, where the adjective "ambisaline" is used to describe an X species so that X^+ and X^- can occur as both cations and anions in isolable salts, although very often not with common counterions.

The department is intensely focused on fluorine chemistry, i.e., on fluorine; therefore, we conducted a literature review on the effects of fluoride on human health in collaboration with researchers from China, Hungary, Spain and Japan. It was confirmed that the only well-defined beneficial effect of fluoride is its protection against dental caries. Excessive intake of fluoride can cause a number of health problems, including dysregulation of G-protein coupled receptors. The effects of increasingly present organofluorine compounds on the health and environment are also poorly understood. The article *Chemical Aspects of Human and Environmental Overload* was published in the prestigious journal Chemical Reviews.

Within the topic of process safety, in 2021 we researched and published work on the introduction of a safe use of liquefied natural gas (LNG) for ship propulsion (European project SUPER-LNG), the relationship between leadership styles and safety management systems in industrial organizations, and resilience and protection of sensitive industrial sites and plants (critical infrastructure) against physical, cybernetic or technology hazards and extreme natural phenomena (European project InfraStress). In addition, we were researching safety challenges in industrial organizations related to the outbreak of the COVID-19 pandemic. We started work on the EU Interreg project TRANSCPEARLYWARNING (TRANSnational Civil Protection EARLY WARNING System) to improve the resilience of ADRION territories to natural and man-made risks.

As always, our department was heavily involved in the field of education and the promotion of science. Members of the department actively participated in the operation of the Jožef Stefan International Postgraduate School, as lecturers or mentors for master's and doctoral students. In addition, the School of Experimental Chemistry maintained its very important relations with primary and secondary schools through experimental lessons conducted at a special laboratory or through direct demonstrations at schools. With the demonstrations of chemical experiments, we participated at the Igraj se z mano/Play with me festival, Znanstival and the Slovenian Science Festival. Some of the activities of the School of Experimental Chemistry were carried out within the framework of the project funded by the JSI and City of Ljubljana. The promotion of science, research and non-formal education was also connected with the European Researchers' Night within the Horizon 2020 programme. At the end of September 2021, we organised and carried out a series of activities within this H2020 project. The workshops of the School of Experimental Chemistry were presented at primary and secondary schools, senior citizens' homes, the library and in the centre of Ljubljana. In the evening, in cooperation with the research departments and centres of the Jožef Stefan Institute, we opened the doors of the Institute in Ljubljana and Podgorica to the public. The visitors were able to see some of the departments and centres, visit the TRIGA nuclear reactor and participate in various workshops.

ERC project

1. H2020 - HiPeR-F; Challenging the Oxidation-State Limitations of the Periodic Table via High-Pressure Fluorine Chemistry
Asst. Prof. Matic Lozinšek
European Commission

Some outstanding publications in the past year

1. J. Han, L. Kiss, H. Mei, A. M. Remete, M. Ponikvar-Svet, D. M. Sedwick, R. Romàn, S. Fustero, H. Morowaki, V. A. Soloshonok, Chemical aspects of human and environmental overload with fluorine, *Chemical Reviews*, 2021, 121, 4678–4742.
2. M. Lozinšek, H. P. A. Mercier, G. J. Schrobilgen, Mixed noble-gas compounds of Krypton(II) and Xenon(VI); [F5Xe(FKrF)AsF6][F5Xe(FKrF)AsF6] and [F5Xe(FKrF)2AsF6][F5Xe(FKrF)2AsF6], *Angewandte Chemie: International edition*, 2021, 60, 8149–8156.
3. A. Kokalj, Ž. Zupanek, M. Tramšek, G. Tavčar, Coordination of a neutral ligand to a metal center of oxo-halido anions: fact or fiction?, *Inorganic Chemistry*, 2021, 60, 11932–11947.
4. E. A. Goreshnik, Influence of the synthetic conditions on a formation of 1-D, 2-D and 3-D copper-chloride coordination polymers, *CrystEngComm*, 2021, 23, 7171–7178.
5. Z. Mazej, E. A. Goreshnik, XeF2 coordination to La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy and Y in rare-earth metal(III) tetrafluoridoborates, *European Journal of Inorganic Chemistry*, 2021, 2669–2681.
6. M. Gerbec, P. Vidmar, G. Pio, E. Salzano, A comparison of dispersion models for the LNG dispersion at port of Koper, Slovenia, *Safety Science*, 2021, 144, 105467-1-105467-16.

Organization of conferences, congresses and meetings

1. Matic Lozinšek, Member of the Organizing Mommittee, Slovenski kemijski dnevi 2021, 22.–24. 9. 2021, Maribor, Slovenia

Awards and Appointments

1. Matic Lozinšek, achievement "The first compounds that simultaneously contain krypton and xenon" was included in the Excellent in Science selection 2021, ARRS

INTERNATIONAL PROJECTS

1. ERC H2020 - HiPeR-F; Challenging the Oxidation-State Limitations of the Periodic Table via High-Pressure Fluorine Chemistry
Asst. Prof. Matic Lozinšek
European Commission
2. H2020 - InfraStress; Improving Resilience of Sensitive Industrial Plants & Infrastructures Exposed to Cyber-Physical Threats, by Means of an Open Testbed Stress-Testing System
Prof. Marko Gerbec
European Commission
3. H2020 - NOCMOC; European Researchers' Night (NIGHT)
Dr. Melita Tramšek
European Commission
4. H2020 - ATHENA; Implementing Gender Equality Plans to Unlock Research Potential of RPOs and RFOs in Europe
Dr. Melita Tramšek
European Commission
5. H2020 - NOCMOC; The Night has its Might, European Researchers' Night (NIGHT)
Dr. Melita Tramšek
European Commission
6. High-Pressure Structural Study of Hydrated Metal Salts of Superweak (B12F12)2- Anion
Asst. Prof. Matic Lozinšek
Slovenian Research Agency

RESEARCH PROGRAMME

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

R & D GRANTS AND CONTRACTS

1. Holistic sustainability evaluation of critical raw materials - closing gaps and developing new methodological approaches
Dr. Robert Kocjančič
2. The quest for high-temperature superconductvity and exotic magnetism in fluoridoargentates(II)
Asst. Prof. Matic Lozinšek
3. Advanced reagents for (asymmetric) nucleophilic fluorination
Asst. Prof. Gašper Tavčar
4. Structures of elusive noble-gas compounds elucidated by 3D electron diffraction
Asst. Prof. Matic Lozinšek
5. High-pressure stabilization and phase transitions of elusive transition-metal fluorides
Asst. Prof. Matic Lozinšek
6. Utilization of secondary lead slag as a secondary raw material for the production of lead
Asst. Prof. Gašper Tavčar
7. Innovative ECO plasma seed treatment (for sowing and for human and animal diet/nutrition)
Asst. Prof. Gašper Tavčar
Ministry of Education, Science and Sport
8. National Air Pollution Control Programme (OP-NEC)
Dr. Robert Kocjančič
Ministry of the Environment and Spatial Planning
9. Consultations and Analyses for Foreign Customers
Prof. Maja Ponikvar-Svet
10. P.439148; Method of Oligomerization of Unsaturated Hydrocarbons
Dr. Zoran Mazej
University of Warsaw

NEW CONTRACT

1. Utilization of secondary lead slag as a secondary raw resource for the production of lead
Asst. Prof. Gašper Tavčar
Th Re-mining d. d.

VISITOR FROM ABROAD

1. Juan D. Forero-Saboya; training and laboratory work, ICMAB-CSIC, Barcelona, Spain, 12.7.2021 - 12.10.2021
2. Dr. Kshitij Gurung and Dr. Peter Brazda; visit Czech–Slovenian cooperation GA

CR-ARRS, Department of Structural Analysis, Institute for Physics, Prague, 8.11.2021 - 18.11.2021

STAFF

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1. Nazariy Pokhodylo, Yurii Slyvka, Evgeny A. Goreshnik, Roman Lytvyn, "Synthesis, crystal structure and Hirshfeld surface analysis of (4-methylphenyl)[1-(pentafluorophenyl)-5-(trifluoromethyl)-1H-1,2,3-triazol-4-yl]methanone", *Acta crystallographica. Section E, Crystallographic communications*, 2021, **77**, 10, 1067-1071.

2. Yurii Slyvka, Nazariy Pokhodylo, Evgeny A. Goreshnik, Olexiy V. Pavlyuk, Marian G. Mys'kiv, "Syntheses and crystal structures of two copper(I)- halide π, ρ-coordination compounds based on 2-[(prop-2-en-1-yl)sulfanyl]pyridine", *Acta crystallographica. Section E, Crystallographic communications*, 2021, **e77**, part 11, 1180-1184.

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4. Matic Lozinšek, Hélène P. A. Mercier, Gary J. Schrobilgen, "Mixed noble-gas compounds of Krypton(II) and Xenon(VI); [$F_5Xe(FKrF)AsF_6$] and [$F_5Xe(FKrF)_2AsF_6$]", *Angewandte Chemie*, 2021, **60**, 15, 8149-8156.

5. Jan Bitenc, Antonio Scafuri, Klemen Pirnat, Matic Lozinšek, Ivan Jerman, Jože Grdadolnik, Bernard Fraisse, Romain Berthelot, Lorenzo Stievano, Robert Dominko, "Electrochemical performance and mechanism of calcium metal-organic battery", *Batteries & supercaps*, 2021, **4**, 1, 214-220.

6. Jianlin Han, Loránd Kiss, Haibo Mei, Attila Márió Remete, Maja Ponikvar-Svet, Daniel Mark Sedgwick, Raquel Romàn, Santos Fustero, Hiroki Moriwaki, Vadim A. Soloshonok, "Chemical aspects of human and environmental overload with fluorine", *Chemical reviews*, 2021, **121**, 8, 4678-4742.

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15. Zoran Mazej, Evgeny A. Goreshnik, "Attempted syntheses of new mixed-cation hexafluoridoarsenates(V) in liquid anhydrous HF acidified with AsF_5; the crystal structures of $A_3M(HF)Mn(AsF_6)_7$($A = H_3O$, K/H_3O M = Ca, Sr, Ba)", *Journal of fluorine chemistry*, 2021, **244**, 109745.

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20. Marko Gerbec, Peter Vidmar, Gianvito Pio, Ernesto Salzano, "A comparison of dispersion models for the LNG dispersion at port of Koper, Slovenia", *Safety science*, 2021, **144**, 105467.

21. Marija Čolović, Metka Hajzeri, Melita Tramšek, Boris Orel, Angelja Kjara Surca, "In situ Raman and UV-visible study of hybrid electrochromic devices with bis end-capped designed trialkoxysilyl-functionalized ionic liquid based electrolytes", *Solar energy materials and solar cells*, 2021, **220**, 110863.

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REVIEW ARTICLE

1. Maja Ponikvar-Svet, Diana N. Zeiger, Joel F. Liebman, "Alkaloids and selected topics in their thermochemistry", *Molecules*, 2021, **26**, 21, 6715.

Short Article

1. Matic Lozinšek, "Nitrosonium tetrafluoridoborate, NOBF$_4$", *IUCrData*, 2021, **6**, x211215.

Independent Component Part or a Chapter in a Monograph

1. Marko Gerbec, Gabriele Giunta, "InfraStress approach on risk modelling of cascading events with live data for decision support", In: *Cyber-physical threat intelligence for critical infrastructures security: securing critical infrastructures in air transport, water, gas, healthcare, finance and industry*, Now Publishers, 2021, 2-21.

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DEPARTMENT OF PHYSICAL AND ORGANIC CHEMISTRY

K-3

The department is focused on investigating physicochemical processes on the surfaces of solids, such as corrosion and heterogeneous catalysis, and the synthesis of new compounds. The synergy of these fields is created in studies of the corrosion protection and functionalisation of materials by introducing an integrative experimental–modelling approach with a combination of experimental electrochemical and surface-analysis techniques and modelling and simulation based on first principles using methods of density functional theory (DFT).

Corrosion is a widespread phenomenon with enormous economic and environmental impacts. The cost of corrosion damage is estimated at €2.5 trillion annually. Due to the enormous costs, protecting metals and alloys is essential. Corrosion protection, with the primary goal being to prolong the lifetime of metallic materials, is one of the ways to reduce the need for steeply increasing production and thus preserve resources for the future. Traditional ways of corrosion protection, such as conversion chromate coatings, can no longer be used due to ecological restrictions. The needs of industry, in particular transportation, construction, machine, and electronics, postulate the requirements for developing efficient, sustainable, and environmentally friendly coatings, which at the same time exhibit additional functional characteristics. Our research work in the field of corrosion protection is devoted to all major surface treatments, such as corrosion inhibitors, conversion coatings, organic coatings, and inorganic coatings (Figure 1), for major metals and alloys, which are indispensable today, such as major lightweight (Al), energy efficient (Cu), and infrastructure (Fe and Zn) materials. Lightweight aluminium alloys and contemporary high-strength steels are used in various applications, especially in the transport industry, where there is a great need to reduce the weight of vehicles and consequently reduce emissions into the environment. Steels and alloys based on copper are indispensable materials in infrastructure, construction and other industries.

In our laboratory we investigate the alternatives mentioned above (Figure 1) and even combine them, e.g., sol-gel coatings and inhibitors, to achieve barrier and active protection, where the coating after the corrosion damage can self-heal. We also introduce modern methodologies in corrosion protection, such as atomic layer deposition (ALD).

We have achieved a major breakthrough in understanding the mechanism of corrosion inhibition with organic compounds by introducing an **integrative** experimental–modelling approach with the combination of experimental electrochemical and surface-analysis techniques, and modelling and simulations based on first principles using methods of density functional theory (DFT). This approach results in a more rational and ecologically oriented use of chemicals, which is in line with the European Union's directives on sustainable development and the circular economy.

2.1. The integrative experimental–modelling approach of novel corrosion inhibitors

In-depth fundamental knowledge of surface processes is needed to design effective corrosion protection because our understanding of the mechanism of corrosion inhibition at the atomic level is still very limited. To overcome this we introduced a synergistic iterative approach that consists of the following three research directions: (1) inorganic and organic synthesis, (2) electrochemical and surface-analysis techniques, and (3) modelling and simulations based on DFT.

Head:
Prof. Ingrid Milošev
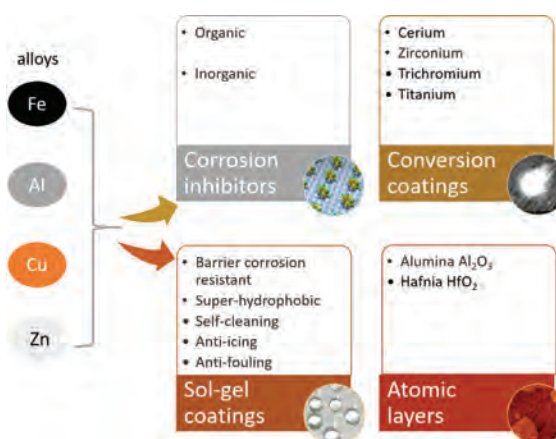
Figure 1: Types of corrosion protection and functionalisation of materials.

Prof. Ingrid Milošev has joined the Editorial Board of the *CORROSION* journal as an Associate Editor. *CORROSION* was started in 1945 by the Association of Materials Protection and Performance (AMPP, former NACE). AMPP is a global community of professionals dedicated to materials protection through the advancement of corrosion control and protective coatings with more than 40,000 members. The *CORROSION* journal, led by Technical Editor in Chief Prof. John Scully, provides a permanent record of progress in the science and technology of corrosion prevention and control, featuring peer-reviewed technical articles from the world's top researchers.

2.1.1. Organic molecules as corrosion inhibitors

We investigated alkyl-based and perfluoroalkyl-based organic compounds as surfactant corrosion inhibitors, whose molecular structures consist of a reactive anchor group and alkyl or perfluoro backbone. The archetypal structure of the investigated organic compounds is presented in Figure 2. We addressed the effect of anchor group and backbone chain on the performance of organic compounds as corrosion inhibitors for aluminium. Different aspects of such systems were investigated: the length of the alkyl chain for a particular anchor group, the effect of the anchor group at a particular length of the alkyl and perfluoroalkyl chains, and the Cl$^-$ penetration into the organic self-assembled monolayer.

The stability of the corresponding organic layer on hydroxylated Al surfaces is given by the strength of the anchor-group adhesion to the surface and lateral cohesion between the backbones (Figure 2a). Among the investigated inhibitors, phosphonic acids are efficient corrosion inhibitors for Al, irrespective of the length of the backbone, which can be attributed to the strong adsorption affinity of the phosphonate anchor group (Figure 2b). Carboxylic acids are also promising inhibitors, but the adsorption affinity of the carboxylate anchor group is considerably lower, and the corresponding organic layer is sufficiently stabilised only with the aid of sufficiently long backbones. Other investigated anchor groups do not show noticeable adsorption affinity, and the corresponding compounds are inefficient for inhibiting the corrosion of Al (Figure 2b). Longer backbones are beneficial for enhancing the corrosion-inhibition efficiency of the investigated organic compounds; however, it can be reasonably anticipated that the size of the backbone should not be too large, or else the solubility of the compound would become too low

Figure 2: Schematic summary of integrative investigations of selected organic compounds as possible corrosion inhibitors for aluminium: (a) archetypal structure of investigated organic compounds, (b) anchor groups, (c) backbone types ordered according to efficiency when anchored with carboxylic group, (d) lateral cohesive interactions and effective coverage for short and long backbone chains, and (e) activation barrier for penetration of Cl$^-$ through adsorbed organic monolayer as a function of organic monolayer thickness.

and the tendency to form micelles too high. According to our experimental and modelling results, for a specific type of chain, longer backbones are generally superior to shorter ones (Figure 2c). However, the efficiency of protection depends on the type of backbone: shorter perfluoroalkyl chains (i.e., Cf8) are superior to shorter alkyl chains (i.e., C8), whereas, for long backbones, the alkyl chains become superior to perfluoroalkyl chains (i.e., C17 > Cf17). This "trend inversion" can be attributed to the interplay between the effective surface coverage and the lateral intermolecular interactions between backbones. For shorter chains, the coverage is greater for perfluoroalkyl chains, whereas for longer chains, the lateral cohesive interactions are superior for alkyl chains. The efficiency of shorter perfluoroalkyl chains can be substantially improved by adding either an alkylene spacer (i.e., Cf8-C3), a benzene spacer (i.e., Cf8-Bn), or an additional perfluoroalkyl chain with a benzene spacer (i.e., (Cf8)$_2$-Bn). Back backbone tilting makes the lateral cohesive interactions stronger, resulting in greater effective coverage for longer backbones (Figure 2d). Long backbones are also more effective at hindering the access of reactive species (i.e., chlorides) to the Al surface (Figure 2e). Notice that the activation barrier for the penetration of Cl$^-$ increases with the thickness of the organic layer up to about 10 Å (here, a full monolayer coverage is assumed, which, according to experiments, for carboxylic acids forms only for long alkyl chains) and then it becomes almost independent of the layer thickness. The role of longer backbones is therefore two-fold, i.e., to stabilise the organic layer and effectively hinder access to the surface of the Al.

The studies were conducted in collaboration with researchers from the CNRS, Chimie ParisTech, France, and Eötvös Loránd University, Institute of Chemistry, Hungary.

2.1.2. Synergistic effect of two corrosion inhibitors

2-mercaptobenzimidazole (MBI or S) and octylphosphonic acid (OPA or P) and their binary mixtures (xS+yP, where x and y are the molar ratios in %) were tested as corrosion inhibitors for Cu and Al in a 3 wt.% NaCl solution using the electrochemical polarisation experiments, whereas the adsorption of the inhibitors was characterised with X-ray photoelectron spectroscopy (XPS) and Fourier transform infrared spectroscopy (FTIR) surface analyses, DFT calculations, and wettability measurements. 90S+10P was found to be superior to 100S (and other mixtures) on Cu, which reveals the synergy between MBI and OPA. XPS data showed that in NaCl without inhibitors, the surface is covered by a Cu(I) oxide layer, whereas in the presence of MBI, a thin protective inhibitor-based layer is formed, and the formation of the Cu(I) oxide is either suppressed or buried beneath the inhibitor layer. DFT calculations reveal that, depending on surface details, MBI can bind to copper surfaces in the thiolate and thione forms, whereas the thiol form can be discarded. XPS nitrogen spectra indeed confirmed that MBI bonds to copper in the thiolate form (pyridine and pyrrole nitrogen present); however, when OPA is also present, XPS analysis reveals that the bonding mechanism changes: in addition to thiolate, also thione forms with pyrrole nitrogen were observed for 90S+10P.

Furthermore, for 90S+10P, a much thicker inhibitor film forms compared to 100S, which exhibits a strong hydrophobic character. Within the film, the MBI molecules are chemisorbed in the first monolayer, followed by multilayers of metallorganic Cu(I)MBI complexes. Stacking layers leads to highly compact structures, which act as an efficient barrier to copper dissolution. Within a narrow pH range of 1 unit (i.e., between pH 3 and 4), the thickness, compactness, and corrosion inhibitive performance of the grown films varies with xS+yP solutions.

On this basis, a tentative mechanism of synergy between dissolution, the formation of soluble species, and adsorption was proposed (Figure 3) depending on the limiting pH (pH$_L$). It is hypothesised that a low pH, pH < pH$_L$ (note that OPA makes the solution acidic), and the presence of chloride ions strongly favour the formation of soluble Cu(II)OPA complexes over adsorption, resulting in the change of activity of the surface that for 90S+10P becomes more prone to adsorption of MBI. Furthermore, in the acidic environment of the MBI+OPA mixture, the activation of the Cu surface is stronger than at the near-neutral pH of the 100S solution. Cu(I) species, formed by Cu dissolution at lower pH (pH$_L$ = 3.5 - 4), thus react with MBI, resulting in the formation of a thick and compact layer. At pH > pH$_L$, a thin layer is formed due to the stable Cu$_2$O and a much lower availability of Cu(I) species to form a complex with MBI at the surface.

In contrast to Cu, binary inhibitor S+P combinations do not act synergistically on Al. Nevertheless, the S+P/Al system is stable in the sense that the presence of the S inhibitor in the S+P mixture does not obstruct the inhibitory ability of P. In addition to 100P, the combination 10S+90P also performs well. Both 100P and 10S+90P form layers with strong hydrophobic characters.

We provided strong evidence that chloride ions play a dual role in forming a micrometre-thick film of polymerised [Cu-Cl-MBI]$_n$. This occurs when the copper is exposed to a 3 wt.% NaCl solution containing 1 mM of the mixture of MBI and OPA, in the molar ratio MBI:OPA of 9:1. The chloride ions act simultaneously as a promoter of polymerised [Cu-MBI]$_n$/[Cu-Cl-MBI]$_n$ film formation and a reactant that is incorporated into the film, as confirmed by the time-of-flight secondary-ion mass spectrometry (ToF-SIMS). Also, the formation of a Cu$_2$O film under the Cu-inhibitor film was proven with focused ion beam microscopy (FIB-SEM), with chemical analysis employed at the cross-section of the thick polymerised film using energy-dispersive X-ray spectroscopy (EDS). The Cu(I) oxide underlayer, together with the porous straw-like morphology of the [Cu-Cl-MBI]$_n$ overlayer, is believed to be responsible for the excellent corrosion protection of copper, even in a chloride environment without the reservoir of MBI+OPA. We also reported a new insight into the mechanism of degradation for the Cu-MBI/Cu-Cl-MBI film that results in forming (MBI)$_2$ dimers. The inhibitor layer, formed in a NaCl solution and containing the synergistic combination of MBI and OPA, showed an outstanding resistance to degradation.

Figure 3: Proposed tentative polymeric structures of Cu–MBI: (a) the non-compact voluminous gelatinous film forms at pH < pH$_L$ (for 10S+90P and 50S+50P at pH 3 and 3.3, respectively), (b) the thick protective film forms at pH 4 for 90S+10P, and (c) for 100S the thin film forms at pH 5.5 (pH > pH$_L$).

2.1.3. Molecular electronic properties and corrosion inhibition

A widespread belief in the literature is that corrosion inhibitors' performance depends on the molecular electronic properties of the inhibitor compounds. Among the popular inferences of this kind is that a good inhibitor should have a low HOMO–LUMO gap, where HOMO stands for the highest occupied molecular orbital and LUMO for the lowest unoccupied molecular orbital. In this context, we critically evaluated the often-used simplistic correlations between the molecular electronic parameters of corrosion inhibitors and their experimentally determined corrosion-inhibition efficiencies for a set of 24 heterocyclic organic compounds tested as corrosion inhibitors for copper in a 3 wt.% NaCl aqueous solution. Twelve different molecular electronic descriptors such as the ionisation potential, electron affinity, HOMO–LUMO gap, and dipole moment were tested, and we showed that none had any noticeable correlation with the inhibition efficiency. Therefore, our results cast serious doubt on the assumption above that such parameters correlate with corrosion-inhibition efficiency. Instead, the focus should be given to more appropriate approaches. Among them, machine-learning (ML) techniques currently have the highest potential to generate reasonably robust and predictive models for screening new corrosion inhibitors. However, the challenge is to provide adequate descriptors because descriptors affect the quality of the ML models much more than the ML algorithm itself. In a subsequent study we indeed showed that, in some cases, it is possible to build more predictive models using a ML approach, where molecular electronic parameters are used among the descriptors.

We also analysed some of the pros and cons of inhibition efficiency as a metric for evaluating the performance of corrosion inhibitors, particularly its nonlinearity issue, and introduced a new metric termed inhibition power that uses the universal logarithmic scale and dimensionless decibel units. This new metric is not susceptible to the nonlinearity problem.

2.2 Corrosion protection using the atomic-layer deposition method
2.2.1. The effect of surface pre-treatment and ALD films composition

Atomic layer deposition (ALD) is a thin-film deposition technique based on the sequential use of a gas-phase chemical process; it is a subclass of chemical vapour deposition. The ALD technique allows the formation of nanoscale coatings, commonly referred to as thin films. However, although they have the potential to be applied as protective thin films on metallic biomaterials, they have, hitherto, seldom been investigated for biomedical purposes. For this reason, the protective properties of alumina and hafnia ALD thin films deposited on cp-Ti as a substrate have been compared in this study.

On June 9, 2021, Prof. Anton Kokalj presented the webinar within the CorroZoom series organised by Prof. G.S. Frankel of The Ohio State University, Columbus, USA. This series hosted six top research scientists from all over the world. Prof. Kokalj's lecture entitled "Molecular modeling of corrosion inhibitors" is currently a hot topic of corrosion research and was devoted to the DFT modelling of the mechanism of adsorption and bonding of organic molecules on metal surfaces.

Before deposition, cp-Ti specimens have been prepared in two ways: grinding, and grinding followed by polishing (Figure 4). Such surfaces have been denoted as rough and smooth, respectively. The thickness, composition, morphology, and topography of alumina and hafnia films have been determined using ellipsometry, FIB-SEM/EDS, ToF-SIMS, and 3D profilometry. A homogeneous, stoichiometric composition of alumina and hafnia was obtained with a layer thickness of aprox. 150 nm. The anti-corrosive properties of ALD thin hafnia (HfO_2) and alumina (Al_2O_3) films were measured in a simulated body fluid solution using electrochemical impedance spectroscopy (EIS) and potentiodynamic polarisation curves. The roughness of the cp-Ti surface plays an essential role in the protective properties of these films, especially those of hafnia. ALD films with better anti-corrosive properties were obtained when deposited on a smooth surface, as evidenced by EIS long-term, 40-day tests. ALD films showed a very low porosity, calculated from the electrochemical parameters, and significantly lower corrosion current densities than bare cp-Ti specimens. Films of hafnia provided lower porosity and slightly better protective properties. On the other hand, according to EIS long-term tests, alumina retained slightly greater impedance values than hafnia. Since both alumina and hafnia are biocompatible materials, this study confirms the possibility of using them to reduce the risk of failure for medical implants made of cp-Ti in a human body.

Figure 4: From left to right: 3D surface profiles of differently prepared bare cp-Ti specimens (ground and polished); SEM images of the cross sections of cp-Ti specimens coated with 150-nm-thick Al_2O_3 and HfO_2 thin films; Potentiodynamic polarisation curves and electrochemical impedance spectra of bare and ALD coated ground and polished, Ti-500 and Ti-OPS, specimens recorded in simulated physiological solution.

2.2.2. Multilayer ALD films

For a thickness of 60 nm, the alumina films were prepared in two configurations (single and multilayer) with hafnia to explore whether adding hafnia is beneficial. ALD films deposited on chemically etched cp-Ti and SS316L are homogenous and compact, as both single and multilayers. The presence of hafnia as an interlayer seems to affect the structure of the multilayers minimally. Some surface dents were noted, as well as agglomerates. Alumina ALD films exhibit good adhesion to polished cp-Ti and SS316L substrates in both single and multilayer combinations with hafnia. AFM combined with SKPFM showed that more positive Volta potential difference values were obtained on the ALD films due to their higher work function and highly insulating properties that strongly inhibit the electron transfer and, in turn, electrochemical interaction at solid/solution interfaces. After 1 hour of immersion in a simulated physiological solution, all three types of ALD films provide significant barrier protection of the underlying substrates, showing reduced current densities by two or three orders of magnitude. However, after 30 days of immersion, it was found that a 20-nm-thick alumina film failed, especially in the case of the cp-Ti substrate.

On the other hand, 60-nm-thick films, either pure alumina or multilayer, retained good barrier properties over the immersion period. Electrochemical behaviour is mainly governed by pores, pinholes, and/or other tiny defects in the coating since the shape of the potentiodynamic curves with and without coatings is more or less the same. The dissolution through the pinholes would be overcome by the repassivation abilities of the substrates. This is especially evident for stainless steel: due to its susceptibility to localised corrosion in chloride-containing solution, the long-term protection becomes an interplay between film porosity and its ability to repassivate through the pores and defects.

Multilayer combination, 60 nm thick, and in configuration 20-nm alumina/20-nm hafnia/20-nm alumina, did not significantly improve the protective properties compared to a single alumina layer of the same thickness, as would be expected considering the much better protective ability of hafnia. Although remaining highly protective,

the hafnia interlayer may destabilise the multilayer film due to some internal stress or incompatibility, possibly due to the tendency to form agglomerates, leading to the mechanical detachment and dissolution of the ALD film resulting in a defect. ALD thin films of alumina or in combination with hafnia, therefore, possess good barrier properties and are proper candidates for use on specific medical implants, but on the condition of ensuring a sufficient film thickness and not being under a mechanical load. The study was conducted in collaboration with researchers from the University of Udine, Italy.

2.3. Hybrid sol-gel coatings used for corrosion protection
2.3.1 Silane-siloxane coatings

The sol-gel synthesis process is a versatile method used to produce a wide variety of materials and is increasingly used as a surface modification method to alter porosity, wettability, catalytic activity, biocompatibility, and the corrosion performance of underlying substrates. Sol-gel coatings remain one of the important fields of our research work. New hybrid silica-acrylic coatings were synthesised by mixing two sols leading to polycondensation: Sol 1 obtained by copolymerisation between MAPTMS (3-(trimethoxysilyl)propyl methacrylate) and acrylate monomers, and Sol 2 of hydrolysed TEOS (tetraethyl orthosilicate). Six monomers with different lengths of the alkyl chain were used (Figure 5). Depending on the acrylate ester derivative used for the reaction, the sols were denoted as siloxane-PXMA, where X stands for the derivative of the acrylate monomer (E ethyl, M methyl, B butyl, H hexyl, O octyl, and D dodecyl). Two triads can be distinguished: short-chain coatings (M1, E2, and B4) with up to four carbon atoms and long-chain coatings (H6, O8, and D12) with up to twelve carbon atoms. The water contact angles increased almost linearly from the coating with a methyl group (60°) to the coating with a butyl group (80°). The contact angles remained unchanged for chain

lengths with more than four carbon atoms. The M1, E2, and B4 coatings exhibited a smooth, nodular morphology. However, the second triad coatings showed silica-rich islands or domains resulting from the inhomogeneous mixing of the two sols due to greater differences between the polar and nonpolar parts. This led to a significantly reduced degree of heterocondensation and preferred cross-linking of the silica species. Due to the inhomogeneous coating structure and composition, the coatings of the second triad exhibited poor corrosion protection. All three coatings were corroded after 1 week of exposure to 3.5 wt.% NaCl.

In the first triad of short-chain coatings, six months of immersion in the saline environment was the least harmful to the coating with ethyl (E2) and butyl (B4) groups, which remained intact. The coating with a methyl group (M1), better known as siloxane-PMMA, exhibited the lowest resistance within the first triad, with the impedance value and the phase angle dropping to half their magnitude in the first 3 months, and then remaining constant for the 3 three months. The superior corrosion resistance of siloxane-PEMA (E2) and -PBMA (B4) coatings was explained by the extremely high values of the pore resistance, which were in the range of 10^{10} W cm^2 after 6 months in 3.5 wt. % NaCl.

A detailed study using ^{29}Si MAS NMR showed that the total degree of condensation and the degree of condensation of the organic part (T species) were reduced for monomers with longer alkyl chains in the structure as a consequence of the steric effect. The highest value for the total degree of condensation of the T species was observed for the E2 and B4 coatings.

The study demonstrated that the siloxane-PMMA (M1) coating, already known to be corrosion resistant, can be further upgraded with different acrylates to improve its corrosion protection (E2, B4).

Siloxane-polyacrylic sol-gel coatings differing in the length of alkyl or perfluoroalkyl chains bonded to the acrylate group were synthesised and deposited on a 7075-T6 aluminium alloy (Figure 6). The degree of copolymerisation between the MAPTMS and the acrylate derivative (i.e., of the organic part) depends on the type of derivative: it increases from methyl to butyl and then reaches a plateau. For derivatives with a longer chain, the steric effect prevents a further increase in copolymerisation kinetics and leads to an uneven polycondensation. The same trend was observed for the hydrophobicity of the coatings: it increases for derivatives with alkyl chains up to four carbon atoms, but longer chains showed no further change in
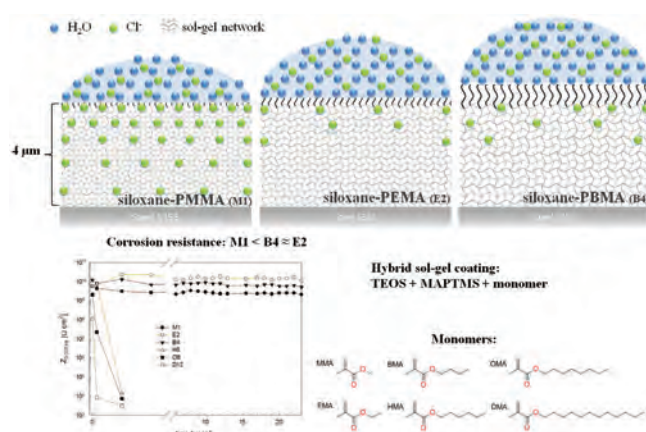
Figure 5: Proposed mechanism for electrolyte uptake/penetration by M1, E2, and B4 coatings. Impedance values at low frequencies are presented as a function of immersion time and the structural formula of six monomers.

hydrophobicity. The replacement of hydrogen with fluorine atoms in the chain enhances the sol's copolymerisation kinetics and increases the coating's hydrophobicity.

The surface and in-depth chemical composition were investigated by XPS, ToF-SIMS, and glow discharge optical emission spectroscopy (GDOES). The coatings are comprised predominantly of an organic part, but an inorganic part with siloxane bonds is essential for achieving good adhesion with the substrate. Positive and negative TOF-SIMS fragments characteristic for alkyl chains at acrylate derivatives were identified, and their intensity depends on the type of derivative. GDOES in-depth profiles confirmed a homogeneous in-depth composition of the coatings with a sharp coating/substrate interface.

The photothermal beam-deflection spectrometry results showed that the coatings with alkyl chains between hexyl and dodecyl exhibited higher porosity than those with shorter chains. Indeed, the corrosion resistance of the coatings with a short chain, specifically ethyl and butyl, shows superior performance in 5 wt.% NaCl solution up to 18 months. Replacing the hydrogen with fluorine atoms does not significantly affect the corrosion resistance.

Another significant result refers to the thermal conductivity and diffusivity of these coatings. Compared to PMMA organic coatings, the inorganic-organic hybrid Si-P*X*MA sol-gel coatings achieve a ca. 50 % higher thermal conductivity and diffusivity. This was explained by the beneficial effect of the siloxane phase in the coating. The sol-gel hybrid methodology, therefore, offers an important route for the modification of thermal properties by a combination of inorganic to organic contents where the former, as an integral part of the coating network, affects the thermal properties without the need for introducing fillers or nanoparticles. Excellent thermal properties combined with strong corrosion protection in a chloride solution are the basis for various applications of these siloxane-polyacrylic coatings. The study was conducted in collaboration with researchers from the CNRS, Chimie ParisTech, France, and the University of Nova Gorica.
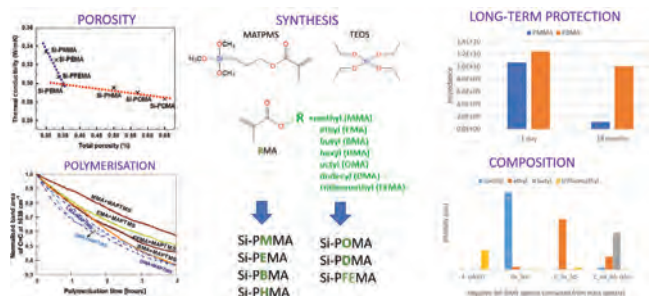
Figure 6: Effect of acrylate monomers in siloxane-silica sol-gel coating (Si-PXMA) on porosity, polymerisation kinetics, impedance values, and coating composition.

2.3.2. Silane-based coatings with zirconia

Two types of acrylic hybrid coatings were synthesised, one containing only Si and the other both Si and Zr. Real-time FTIR data showed the essential differences in the formation of acrylic coatings based on Si (TM coating), and Si and Zr (TMZ coating). These differences are associated with the intensity of the bands ascribed to Si–O–Si in Si-based TM coating and Si–O–Si, Zr–O–Zr, and Si–O–Zr bonding in Si/Zr-based TMZ coating (Figure 7). The SEM images of the top view confirmed that both sol-gel coatings formed a continuous, smooth surface without any cracks. The coatings were 2–3 micrometres thick without any visible pores or defects. The EIS analyses showed that both coatings provided barrier properties at the beginning of the immersion in 0.1-M NaCl solution. However, after prolonged immersion, the Si/Zr-based coating still provided barrier protection, whereas the Si-based coating lost barrier properties after a few days of immersion. The degradation of the coatings was additionally confirmed by XPS analysis. Comparing the high-resolution XPS spectra of the Si/Zr-based coating before and after immersion confirmed the unchanged spectra of Si, O, C, and Zr. On the other hand, XPS spectra of the Si-based coatings show the presence of aluminium corrosion products (peaks for Al and Cl detected), which diffused through the coating. The difference in the corrosion resistance of both coatings was also confirmed in the salt-spray chamber, where the Si/Zr-based coating remained stable for more than 500 hours (Figure 8).

The results provide a valuable demonstration of the correlation between EIS and XPS data and are crucial to showing evidence for the distribution of the aluminium corrosion products and coating degradation. Better barrier corrosion protection and lower coating degradation on the aluminium surface were achieved with a Si/Zr-based hybrid coating. Therefore, Si/Zr-based hybrid coatings prepared under optimised conditions can be considered important candidates for the replacement of chromate-based treatments for Al-based materials. The study was conducted in collaboration with researchers from the CNRS, Chimie ParisTech, France.
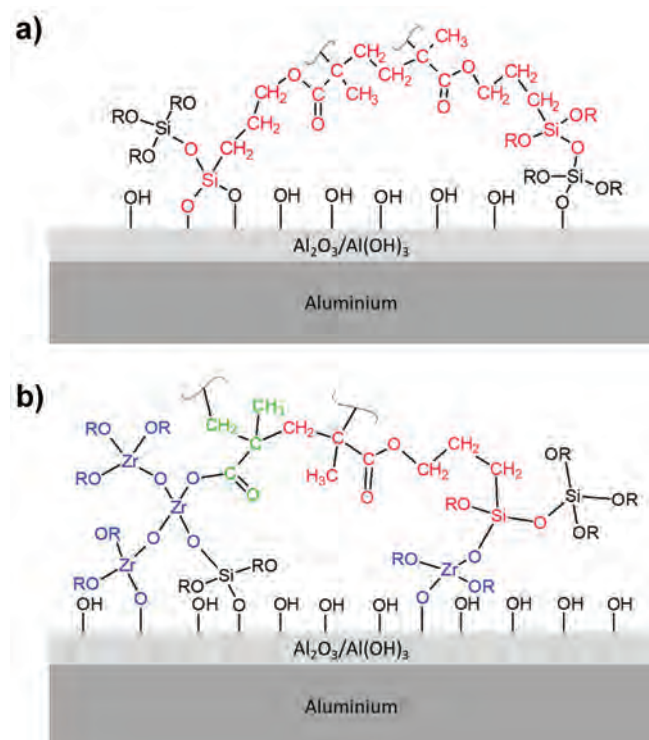
Figure 7: Schematic presentation of the sol-gel network in (a) TM and (b) TMZ coatings deposited on the aluminium surface.

2.3.3. Hybrid sol-gel coatings with active corrosion ability

In collaboration with researchers from the Technical University of Delft, The Netherlands, Vrije University of Brussels, Belgium, and Complutense University of Madrid, Spain, we worked on the effect of the pre-treatment on the sol-gel application. Silane sol-gel films deposited on aluminium and aluminium alloys have been widely studied as chemical conversion coatings and coupling agents between the substrate and organic layers. This study sought to investigate the effect of the surface chemical treatment before sol-gel application on the interfacial adhesion properties of a hybrid sol-gel film. Different surface pre-treatments, including two abrasive treatments and three chemical surface pre-treatments, were used, and their effects on surface chemistry and surface roughness were assessed. Surfaces were characterised by SEM, XPS, roughness measurements, and static contact-angle measurements. Cerium nitrate-loaded hybrid sol-gel films were deposited, and adhesion on commercially pure aluminium was evaluated using pull-off testing. Statistical analysis revealed that, although the highest adhesion values were obtained on rougher surfaces, the strongest correlation exists between the surface hydroxyl fraction and the adhesion strength.

Figure 8: Surface appearance of ground aluminium and coated with TM and TMZ coatings at various exposure times in the salt-spray chamber. The arrows mark the spots where corrosion starts on the aluminium and aluminium coated with TM. The X-cross scribe was made before exposure to salt spray to simulate the coating defect. Testing was performed in 5 wt.% NaCl at 37 °C according to the standard ASTM B117.

The presence of an anodic film and hybrid sol-gel coating loaded with corrosion inhibitors was evaluated as a strategy for the enhanced barrier and active corrosion protection of aluminium alloy 2024-T3. AA2024-T3 specimens were anodised in a modified sulfuric-citric acid bath (SCA) as the first layer of a corrosion-protective multilayer system and subsequently protected by the application of silica-based hybrid sol-gel coatings. These coatings were doped with $LiNO_3$ and $Ce(NO_3)_3$ as corrosion inhibitors and studied in comparison with the inhibitor-free sol-gel coating in terms of morphology, composition, and the corrosion protection of intact and scribed specimens. The anodised AA2024-T3 with an overlaying inhibitor-free sol-gel coating showed the highest impedance modulus during long-term immersion in a 0.1 M NaCl aqueous solution. Adding Li- and Ce-based salts into the hybrid sol-gel formulation showed active corrosion protection compared to the inhibitor-free scribed hybrid sol-gel coating. The Ce-doped sol-gel coating showed less visible corrosion and higher active corrosion protection than the Li-containing one during the long-term immersion test in 0.5 M NaCl. The present findings reveal that the combination of the anodic/hybrid sol-gel layers on AA2024-T3 enhances the corrosion-protection barrier properties of both stand-alone systems, and the incorporation of Li- and Ce-based inhibitors provide active corrosion.

Some outstanding publications in the past year

1. Kokalj A, Lozinšek M, Kapun K, Taheri P, Neupane Sh, Losada-Pérez P, Xie C, Stavber S, Crespo D, Renner FU, Mol A, Milošev I, Simplistic correlations between molecular electronic properties and inhibition efficiencies: Do they really exist? *Corros. Sci.,* 2021, **179**, 108856

2. Milošev I, Kokalj A, Poberžnik M, Carrièrre Ch, Zimerl D, Iskra J, Nemes A, Szabó D, Zanna S, Seyeux A, Costa D, Rábai J, Marcus P, The effects of perfluoroalkyl and alkyl backbone chains, spacers, and anchor groups on the performance of organic compounds as corrosion inhibitors for aluminum investigated using an integrative experimental-modeling approach*, J. Electrochem. Soc.,* 2021, **168**, 071506

3. Spajić I, Rodič P, Šekularac G, Lekka M, Fedrizzi L, Milošev I, The effect of surface preparation on the protective properties of Al_2O_3 and HfO_2 thin films deposited on cp-titanium by atomic layer deposition, *Electrochim. Acta,* 2021, **366**, 137431

4. Kozlica Dž K, Kokalj A, Milošev I, Synergistic effect of 2-mercaptobenzimidazole and octlyphosphonic acid as corrosion inhibitors for copper and aluminium - An electrochemical, XPS FTIR and DFT study, *Corros. Sci.,* 2021, **182**, 109082

5. Rodič P, Zanna S, Milošev I, Marcus P, Degradation of sol-gel acrylic coatings based on Si and Zr investigated using electrochemical impedance, infrared and X-ray photoelectron spectroscopies, *Front. Mater.*, 2021, **8**, 756447

6. Kokalj A, Costa D, Model study of penetration of Cl⁻ ions from solution into organic self-assembled-monolayer on metal substrate. *J. Electrochem. Soc.*, 2021, **168**, 071508

Organization of conferences, congresses and meetings

1. MaX e-School on Advanced Materials and Molecular Modelling with Quantum ESPRESSO (live streamed on YouTube) took place from 17 to 28 May 2021. The e-School was organised by SISSA and ICTP in collaboration with various international institutions, including CINECA, CECAM, Jožef Stefan Institute, Arnes, and University of Shanghai, all under the auspices of MaX CoE and Quantum ESPRESSO Foundation. The school introduced students and young researchers to materials and molecular modelling with Quantum ESPRESSO, covering basic concepts, recent advances and developments, with an emphasis on density functional theory (DFT) and high-performance computing (HPC). The e-School received **a record number of applications** among the ICTP schools: almost **1300** requests arrived from 92 countries for the 120 places available.

Awards and Appointments

1. Matjaž Dlouhy, first prize in the category best student lecture entitled "*The effect of corrosion relevant species on the adsorption of imidazole on copper*", at the 27th annual meeting of the Slovenian Chemical Society entitled "Slovenian Chemical Days 2021", September 22-24, 2021.

INTERNATIONAL PROJECTS

1. COST CA17126: Towards Understanding and Modelling Intense Electronic Excitation
   Prof. Anton Kokalj
   Cost Association
2. H2020 - mCBEEs; Advanced Integrative Solutions to Corrosion Problems Beyond Micro-Scale: Towards Long-Term Durability of Miniaturized Biomedical, Electronic and Energy Systems
   Prof. Ingrid Milošev
   European Commission
3. H2020 - MAMI; Magnetics and Microhydrodynamics - From Guided Transport to Delivery
   Prof. Ingrid Milošev
   European Commission
4. H2020 - ATHENA; Implementing Gender Equality Plans to Unlock Research Potential of RPOs and RFOs in Europe
   Prof. Ingrid Milošev
   European Commission
5. DCOIN: Disentagling COrrosion and its INhibition
   Dr. Matic Poberžnik
   Slovenian Research Agency

RESEARCH PROGRAMMES

1. Chemistry for sustainable development
   Asst. Prof. Peter Rodič

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

R & D GRANTS AND CONTRACTS

1. Multidisciplinary approach towards development of a novel multifunctional heterogeneous catalyst for efficient conversion of H_2 and CO_2 gas mixtures into fuel additives and surrogates
   Prof. Anton Kokalj
2. Development of advanced nanostructured catalysts for hydrogenation of carbon dioxide to methanol
   Prof. Anton Kokalj
3. Structures of elusive noble-gas compounds elucidated by 3D electron diffraction
   Prof. Anton Kokalj
4. Photocatalytic water treatment - development of immobilized catalysts and compact reactor systems
   Asst. Prof. Peter Rodič
5. Ecology laboratory with mobile unit
   Asst. Prof. Peter Rodič
   Ministry of Defence

VISITORS FROM ABROAD

1. Dr Emilie Gaudry, Institut Jean Lamour, University of Lorraine, Nancy, France, 2. 8. – 6. 8. 2021
2. Thiago Trevizam Dorini, Institut Jean Lamour, University of Lorraine, Nancy, France, 2. 8. – 12. 8. 2021
3. Dr Florian Brix, Institut Jean Lamour, University of Lorraine, Nancy, France, 2. 8. – 6. 8. 2021

STAFF

Researchers
1. Prof. Anton Kokalj
2. **Prof. Ingrid Milošev, Head**
3. Asst. Prof. Peter Rodič
Postdoctoral associates
4. *Dr. Matic Poberžnik, on leave since 01.01.21*
5. *Dr. Gavrilo Šekularac, on leave since 01.01.21*
Postgraduates
6. Matjaž Dlouhy, B. Sc.

7. Lea Gašparič, B. Sc.
8. Erik Gregori, B. Sc.
9. Dževad Kozlica, M. Sc.
10. Ana Kraš, M. Sc.
11. Nikolina Lešić, M. Sc.
12. Ivan Spajić, M. Sc.
Technical officer
13. Barbara Kapun, B. Sc.

BIBLIOGRAPHY

ORIGINAL ARTICLE

1. Njomza Ajvazi, Stojan Stavber, "Direct cross-coupling of alcohols with O-nucleophiles mediated by N-iodosuccinimide as a precatalyst under mild reaction conditions", *Catalysts*, 2021, **11**, 7, 858.

2. Anton Kokalj *et al.* (12 authors), "Simplistic correlations between molecular electronic properties and inhibition efficiencies: do they really exist?", *Corrosion science*, 2021, **179**, 108856.

3. Anton Kokalj, "On the alleged importance of the molecular electron-donating ability and the HOMO-LUMO gap in corrosion inhibition studies", *Corrosion science*, 2021, **180**, 109016.

4. Dževad Kozlica, Anton Kokalj, Ingrid Milošev, "Synergistic effect of 2-mercaptobenzimidazole and octylphosphonic acid as corrosion inhibitors for copper and aluminium: an electrochemical, XPS, FTIR and DFT study", *Corrosion science*, 2021, **182**, 109082.

5. Anton Kokalj, "Molecular modeling of organic corrosion inhibitors: calculations, pitfalls, and conceptualization of molecule-surface bonding", *Corrosion science*, 2021, **193**, 109650.

6. Anton Kokalj, Chenyang Xie, Ingrid Milošev, Daniel Crespo, "How relevant are molecular electronic parameters for predicting corrosion inhibition efficiency: imidazoles as corrosion inhibitors of Cu/Zr materials in NaCl solution", *Corrosion science*, 2021, **193**, 109900.

7. Ivan Spajić, Peter Rodič, Gavrilo Šekularac, Maria Lekka, Lorenzo Fedrizzi, Ingrid Milošev, "The effect of surface preparation on the protective properties of Al_2O_3 and HfO_2 thin films deposited on cp-titanium by atomic layer deposition", *Electrochimica Acta*, 2021, **366**, 137431.

8. Peter Rodič, Maria Lekka, Francesco Andreatta, Ingrid Milošev, Lorenzo Fedrizzi, "The synergistic effect of cerium acetate and sodium sulphate on corrosion inhibition of AA2024-T3 at various temperatures", *Electrochimica Acta*, 2021, **370**, 137664.

9. Peter Rodič, Sandrine Zanna, Ingrid Milošev, Philippe Marcus, "Degradation of sol-gel acrylic coatings based on Si and Zr investigated using electrochemical impedance, infrared and X-ray photoelectron spectroscopies", *Frontiers in materials*, 2021, **8**, 756447.

10. Anton Kokalj, Žiga Zupanek, Melita Tramšek, Gašper Tavčar, "Coordination of a neutral ligand to a metal center of oxohalido anions: fact or fiction?", *Inorganic chemistry*, 2021, **60**, 16, 11932-11947.

11. Chenyang Xie, Ingrid Milošev, Frank Renner, Anton Kokalj, Pere Bruna, Daniel Crespo, "Corrosion resistance of crystalline and amorphous CuZr alloys in NaCl aqueous environment and effect of corrosion inhibitors", *Journal of alloys and compounds*, 2021, **879**, 160464.

12. Boštjan Žener, Lev Matoh, Peter Rodič, David Škufca, Ester Heath, Urška Lavrenčič Štangar, "Removal of 18 bisphenols co-present in aqueous media by effectively immobilized titania photocatalyst", *Journal of environmental chemical engineering*, 2021, **9**, 6, 106814.

13. Matevž Topolovec, Ingrid Milošev, Andrej Cör, "Outcome after two sequential revision hip arthroplasties for CoC bearing Fracture with 10 years follow-up: a case report", *Journal of orthopaedic case reports*, 2021, **11**, 7, 45-48.

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15. Shova Neupane *et al.* (11 authors), "Study of mercaptobenzimidazoles as inhibitors for copper corrosion: down to the molecular scale", *Journal of The Electrochemical Society*, 2021, **168**, 5, 051504.

16. Ingrid Milošev, Anton Kokalj *et al.* (13 authors), "The effects of perfluoroalkyl and alkyl backbone chains, spacers, and anchor groups on the performance of organic compounds as corrosion inhibitors for aluminum investigated using an integrative experimental-modeling approach", *Journal of The Electrochemical Society*, 2021, **168**, 7, 071506.

17. Anton Kokalj, Dominique Costa, "Model study of penetration of Cl^- ions from solution into organic self-assembled-monolayer on metal substrate: Trends and modeling aspects", *Journal of The Electrochemical Society*, 2021, **168**, 7, 071508.

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19. Thiago T. Dorini, Florian Brix, Corentin Chatelier, Anton Kokalj, Émilie Gaudry, "Two-dimensional oxide quasicrystal approximants with tunable electronic and magnetic properties", *Nanoscale*, 2021, **13**, 24, 10771-10779.

20. Shova Neupane *et al.* (13 authors), "A model study on controlling dealloying corrosion attack by lateral modification of surfactant inhibitors", *npj Materials degradation*, 2021, **5**, 29.

21. Damir Hamulić, Peter Rodič, Ingrid Milošev, "The influence of length of alkyl chain on the chemical structure and corrosion resistance of silica-polyacrylic hybrid coatings on structural steel", *Progress in organic coatings*, 2021, **150**, 105982.

22. Ruben del Olmo, Urša Tiringer, Ingrid Milošev, Peter Visser, Raul Arrabal, Endzhe Matykina, Johannes M. C. Mol, "Hybrid sol-gel coatings applied on anodized AA2024-T3 for active corrosion protection", *Surface & coatings technology*, 2021, **419**, 127251.

23. Urša Tiringer, Joost Pieter Bernard van Dam, Shoshan Abrahami, Herman A. Terryn, Janez Kovač, Ingrid Milošev, Johannes M. C. Mol, "Scrutinizing the importance of surface chemistry versus surface roughness for aluminium/sol-gel film adhesion", *Surfaces and interfaces*, 2021, **26**, 101417.

SHORT ARTICLE

1. Dževad Kozlica, Ingrid Milošev, "Technical note: Does Cr^{6+} really exist? Difference between charge and oxidation state and how to record them", *Corrosion*, 2021, **77**, 7, 696-699.

INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Bojan Božič, Klara Čebular, Stojan Stavber, "Metal-free and acid-free activation of carbonyl moiety using molecular Halogens or N-halamines", In: *Advances in organic synthesis*, 2021, **15**, 1-97. [COBISS.SI-ID 83022339

2. Ingrid Milošev, Vesna Levašič, Simon Kovač, Tarvo Sillat, Sannakaisa Virtanen, Veli-Matti Tiainen, Rihard Trebše, "Metals for joint replacement", In: *Joint replacement technology*, (Woodhead publishing series in biomaterials), Elsevier, 2021, 65-122.

ENCYCLOPAEDIA, DICTIONARY, LEXICON, MANUAL, ATLAS, MAP

1. Vesna Levašič, Ingrid Milošev, Rihard Trebše, *Angleško-slovenski slovar ortopedskih izrazov*, (Termania), Amebis, 2021.

ELECTRONIC CERAMICS DEPARTMENT

K-5

The Electronic Ceramics Department is active in the research of the synthesis, properties and applications of ceramic materials for electronics and energetics, mainly complex multifunctional materials and structures that can perform multiple functions (multifunctional materials). The materials of interest include piezoelectrics, ferroelectrics, relaxors, multiferroics, conductive oxides, low-dimensional magnets and cuprate superconductors. The emphasis is on the creation of properties by the synthesis and structure on the nano-, micro- and macro-levels. The group also works on the principles of basic technologies for ceramic pressure sensors, ceramic MEMS and flexible electronics.

Head:
Prof. Barbara Malič

We continued with the work on **lead-free piezoelectrics**. In collaboration with colleagues from the Technical University of Darmstadt, Germany, we studied the uniaxial deformation of the ferroelectric $KNbO_3$ single crystal in [010] and [101] orientations at room temperature. The mechanical dislocation and ferroelectric domain structure were investigated using piezo-response force microscopy (PFM). The results suggest that the dislocations act as nucleation and pinning sites for the ferroelectric domains, leading to a local increase in the density of the ferroelectric domain walls.

We continued with the work on **polycrystalline $BiFeO_3$**. We performed a comparative study of uncharged and charged domain walls (DWs) in $BiFeO_3$ ceramics from the point of view of the atomically resolved strain and structure using scanning-transmission electron microscopy. We showed that the uncharged {100}pseudo cubic (pc)-type DWs have a larger associated lattice strain than the charged-"tail-to-tail" {100}pc-type DWs, and we were able to explain the result as a pure intrinsic lattice mismatch. As the {100}pc-type DWs have been experimentally shown to be intrinsically different in strain distribution and structure, we assume that their role in the switching mechanism will be different, depending on their particular strain and charged state.

Together with colleagues from the Norwegian University of Science and Technology, Trondheim, Norway, we published a review paper on the alternating-current (AC) properties of domain walls, which includes our work on $BiFeO_3$ ceramics, in particular the implications of the domain-wall conductivity in the emergent macroscopic piezoelectric response.

In collaboration with colleagues at the National Institute of Chemistry, EPFL, Lausanne, Switzerland, Materials Center Leoben, Austria, and the Tokyo Institute of Technology, Japan we conducted an atomic resolution study using aberration-corrected scanning transmission electron microscopy complemented by Raman spectroscopy and directly revealed, visualized, and quantitatively described static 2–4-nm polar nanoclusters in the nominally nonpolar cubic phases of **barium titanate-based ceramics**. These results helped us understand the atomic-scale structure of disordered materials and may help clarify ambiguities about the dynamic-versus static nature of nano-sized clusters [Figure 1].

$(Na_{1/2}Bi_{1/2})TiO_3$–$BaTiO_3$ (NBT-BT) lead-free piezoceramics are of interest for high-power piezoelectric applications where the hardening of the electromechanical response is of paramount importance. In collaboration with colleagues from Technical University Darmstadt, Germany, we conducted a study on NBT-BT ceramics aimed at identifying the hardening efficiency of the so-called composite approach. The approach consists of dispersing second-phase inclusions, in this case ZnO, in the ceramics to provide pinning effects and thus reduce the domain-wall displacements and the associated losses. With the support of higher harmonic polarization measurements, performed in our lab, we were able to explain the superior thermal stability of the mechanical quality factor in NBT-BT/ZnO composites as a consequence of robust mechanical pinning effects provided by the inclusions.
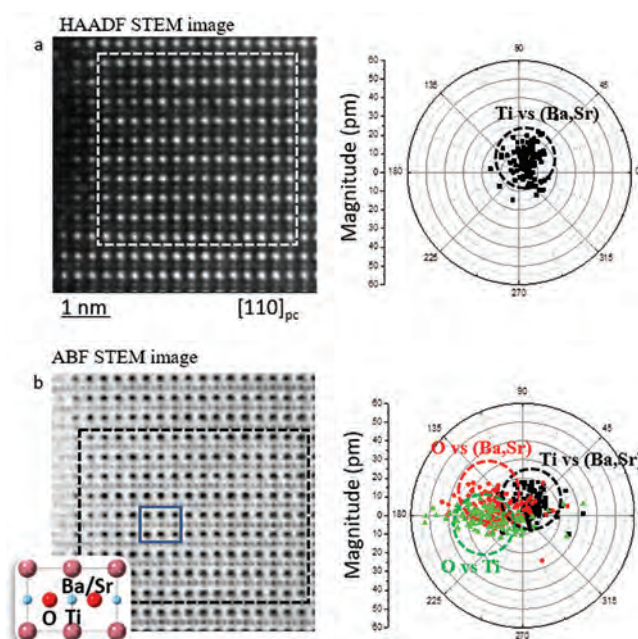
Figure 1: High-angle annular dark-field (HAADF) and annular bright-field (ABF) STEM image of $Ba_{0.6}Sr_{0.4}TiO_3$ in [110] zone axis with corresponding Ti vs (Ba, Sr), O vs (Ba, Sr), and O vs Ti displacements presented in the form of polar plots. The inset in b shows the perovskite unit cell viewed along [110] axis. Dashed rectangles mark areas where displacements were determined. Dashed circles mark areas where majority of the individual types of displacements are present. Displacements of cations and anions do not coincide, indicating non-cubic structure.

In collaboration with colleagues from Friedrich-Alexander-University Erlangen-Nürnberg, Germany, we used piezoforce microscopy (PFM) and transmission electron microscopy to investigate the domain structure of $(Na_{1/2}Bi_{1/2})$ TiO_3 ceramics. Ferroelectric domain switching was observed by applying a sufficiently large electric field, no change in domain configuration was observed in the samples subjected to uniaxial compressive stresses up to 750 MPa.

In ferroelectrics, the mechanisms of hardening by acceptor doping are commonly associated with domain-wall pinning effects provided by oxygen vacancies. In **lead-based relaxor ferroelectrics**, these mechanisms are complicated by the nano-polar structure of these materials and their dynamic contribution to the electromechanical properties. To shed light on this issue, we systematically investigated the hardening effects by Mn doping in $Pb(Mg,Nb)O_3$-$PbTiO_3$ (PMN-PT). We found that the oxygen-vacancies-related pinning manifests similarly both in the ergodic and non-ergodic relaxor phases of the PMN-PT. By reducing the freezing temperature, Mn doping was found to be an efficient approach to improving the thermal stability of the electrocaloric response.

Poling-field-induced changes in the PMN–PT relaxor ferroelectric ceramics around the morphotropic phase boundary (MPB) were investigated, with a detailed examination of the effects of the poling procedure on the piezoelectric and dielectric response, as well as the response of the crystal lattice and the ferroelectric domains. We found that AC poling on the monoclinic (M) side of the phase diagram is more effective than DC poling from the point of a much lower AC field being needed to obtain a similar d33 response as with DC poling. This result was supported by in-situ XRD measurements of the 30 PT M composition, which show a large-strain response at significantly lower AC than the DC field. Furthermore, the Cm M phase possesses low-angle nanodomain walls and exhibits a gradual "cascade-like" motion of the domain walls that starts immediately at low fields ($\sim$2 kV/cm) and saturates roughly at 15 kV/cm, contributing to large strains in the material. The tetragonal-like M phase, however, shows sudden domain switching roughly at the coercive field, with no obvious lattice strain up to 30 kV/cm.

In collaboration with colleagues from the Condensed Matter Department, JSI, and from the Technical University Darmstadt, Germany, we investigated **the electrocaloric (EC) properties** of $0.9Pb(Mg_{1/3}Nb_{2/3})O_3$–$0.1PbTiO_3$ (PMN-10PT) ceramics prepared by the conventional columbite route and mechanochemical synthesis. The samples were able to withstand DC electric fields up to 115 kV/cm, resulting in very high EC temperature changes (ΔT_{EC}) of 2.37 K at 107 °C. In contrast, the ceramics prepared by the columbite route could only withstand $\sim$60 kV/cm and therefore exhibited a much lower ΔT_{EC}. A detailed examination of the microstructure revealed that the respective samples contained a semi-crystalline secondary phase at the triple junctions of the grains, which presumably provided an easy pathway for current propagation. In contrast, in the PMN-10PT obtained by mechanochemical synthesis, the grain boundaries were clean and MgO inclusions were identified. These microstructural features contributed to a higher electrical breakdown field of the ceramics.

Figure 2: Multifunctional cantilevers as working elements in solid-state cooling devices: microstructures of the sandwich-like structure of cantilevers in cross-section, consisting of two $Pb(Mg,Nb)O_3$ ceramic layers and platinum, sintered at different temperatures. When an electric field (E) is applied to the upper ceramic layer, the cantilever bends, as shown schematically in the bottom inset. Experimental setup for testing the proof-of-concept device with cantilevers arranged in a cascade structure is shown on the right.

Despite the challenges of practical implementation, EC cooling remains a promising technology because of its good scalability and high efficiency. To provide a further step in this application area, we fabricated multifunctional cantilever structures made of relaxor ferroelectric PMN-PT, which were stacked in a cascade, forming a proof-of-concept device. Functional testing of the structure revealed that the key element of the device's performance is the poor heat transfer through the cantilever contacts. The study thus clearly showed that further engineering will have to be focused on lowering the thermal contact resistance for an efficient EC operation of the cantilever cascade [Figure 2].

Together with collaborators from McMaster University, Canada, Oakridge National Laboratory in the US, and ANSTO's Australian Synchrotron, we continued the research on **cuprate superconductors**, $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ (Nd-LSCO). We first used resonant X-ray scattering to measure the evolution of electronic nematicity and charge density wave order with hole doping. We found that electronic nematicity – a rotational symmetry breaking of the electronic structure – is associated with the onset of the pseudo-gap phase. Nd-LSCO exhibits a substantial decrease in electronic nematicity, either by increasing the temperature to the onset of the pseudo-gap phase or by increasing the doping through the pseudo-gap quantum critical point.

Moreover, using elastic and inelastic neutron scattering measurements on single crystals of x = 0.125, 0.19, 0.24, and 0.26 we showed that two-dimensional, quasistatic, parallel spin stripes have an onset at temperatures such that the parallel spin stripe phase extends beyond $p*$ and envelops the entirety of the superconducting ground states

in this system. Our measurements of 2D TN and the onset of 2D parallel stripes at optimal and high hole-doping levels in Nd-LSCO, allowed us to complete the phase diagram for 2D parallel stripes and examine their relation to superconductivity.

In the framework of our studies on **low-dimensional magnetism**, we continued our investigations of **manganates**. We performed the synthesis, structural and magnetic characterisation of the $Ba_{1-x}La_{1+x}MnO_{4+\delta}$ ($0 \leq x \leq 0.5$) series. We found that each member of the $Ba_{1-x}La_{1+x}MnO_{4+\delta}$ series exhibits the same spin-glass behaviour previously found in the $x = 0.2$. Moreover, Tg varies with x reaching a maximum of 26.4(4) K for $x = 0.20$ [Figure 3].

Furthermore, using X-ray absorption near-edge structure (XANES) studies we found out that the oxidation state of Mn in the $Ba_{1-x}La_{1+x}MnO_{4+\delta}$ samples varies with x: for $x \leq 0.2$ Mn is in +3.0(1) oxidation state only, whereas a mixed +2/+3 oxidation state was found for $x > 0.2$. The origin of the spin-glass state in the $Ba_{1-x}La_{1+x}MnO_{4+\delta}$ series shows two regimes depending on the oxidation state of the Mn.

In collaboration with the Department of Advanced Materials, JSI, we investigated the relaxor ferroelectric domain structure in the epitaxial $0.67Pb(Mg_{1/3}Nb_{2/3})O_3$–$0.33PbTiO_3$ (PMN-33PT) films on different substrates. PFM analysis was used to show that the domain structure of PMN-33PT films is sensitive to the compressive strain induced in the films. A relaxor-like behaviour was observed at a strain state below 1.1%, while irregularly shaped ferroelectric domains were observed at a higher compressive strain (> 1.9%). The results suggest that epitaxial strain engineering could be an effective approach to tailor and improve the functional properties of **relaxor ferroelectric thin films**.

Patterning of nanostructures of functional-oxide materials by inkjet printing of solution-based inks was studied with colleagues from the Condensed Matter Physics Department, JSI, Faculty of Mathematics and Physics, University of Ljubljana, and CENN Nanocenter. The importance of contact line mobility– either pinned or mobile – on the deposit morphology, either dome-like, flat or ring-like, was addressed. By adjusting the ink solvent composition and controlling the substrate wetting behaviour, deposits with a uniform thickness in the nanometre range could be printed.

Within the field of chemical solution deposition of lead-free ferroelectric thin films our focus was on barium-titanate-based solid solutions with an enhanced ferro- and piezoelectric response.

We continued the research of **thick films** of environmentally benign piezoelectrics based on $K_{0.5}Na_{0.5}NbO_3$ on ceramic substrates for energy harvesting and ultrasound transducer applications. The research was conducted within the Proteus project in collaboration with researchers from the University of Tours, France.

We studied how sintering in different atmospheres affects the structural, microstructural, and functional properties of ~30-μm-thick films of $K_{0.5}Na_{0.5}NbO_3$ (KNN) modified with 0.38 mol% $K_{5.4}Cu_{1.3}Ta_{10}O_{29}$ and 1 mol% CuO. The films were **screen printed** on platinized alumina substrates and sintered at 1100 °C in oxygen or in the air with or without the packing powder. Thick films sintered in oxygen exhibit a piezoelectric d_{33} coefficient of 64 pm/V and an effective thickness coupling coefficient k_t of 43%, as well as very low mechanical losses of less than 0.5%, making them promising candidates for lead-free piezoelectric energy-harvesting applications. The study was conducted in collaboration with researchers from the University of Tours, France.

We continued with the preparation of **thick films using an aerosol deposition method**. The aerosol deposition system is a part of the Laboratory for the Ultracool Preparation of Complex Oxides, for which the financial support was granted by **the Director's fund ULTRACOOL project**. We focused on optimization of processing parameters of functional $0.9Pb(Mg_{1/3}Nb_{2/3})$
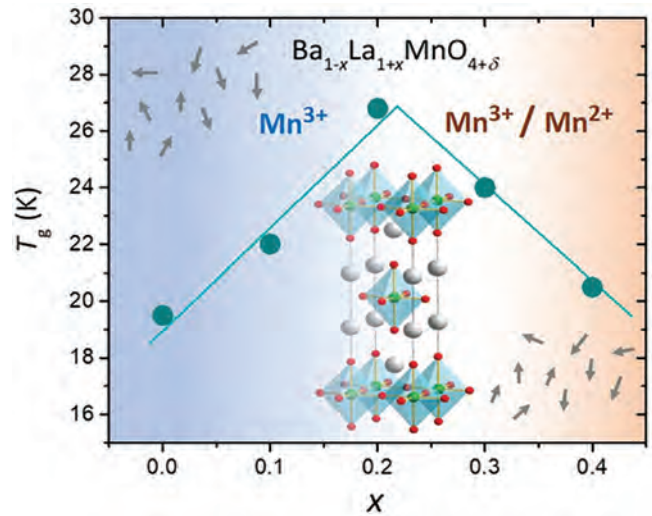
Figure 3: $Ba_{1-x}La_{1+x}MnO_{4+\delta}$ ($0 \leq x \leq 0.4$) series exhibits a rare anisotropic spin-glass behaviour. The freezing temperature, T_g, varies with x, reaching a maximum of 26.4(4) K for x = 0.20. The oxidation state of Mn is also dependent on x.

Prof. dr. Mojca Otoničar and Prof. dr. Tadej Rojac were awarded 'Excellent in science' by the Slovenian research agency in the field of electronic components and materials, for disclosing the influence of polar disorder on the response dynamics of ferroelectric materials. The results of this study were published in the prestigious international journal Advanced Functional Materials.
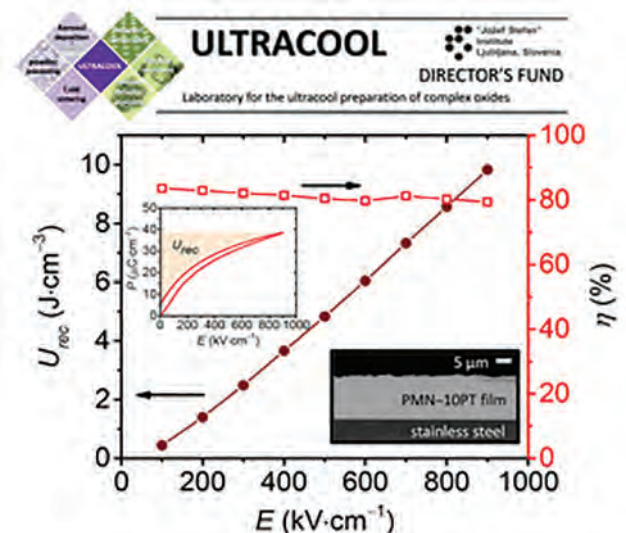
Figure 4: Room temperature energy storage properties of PMN-10PT thick films deposited on stainless steel; recoverable energy density (U_{rec}) and efficiency (η) as a function of electric field (E). Inset (bottom): microstructure of the sample in cross-section taken with a scanning electron microscope. Inset (top): Measurement of polarization (P) as a function of E.

O_3–$0.1PbTiO_3$ (PMN-10PT) thick films deposited on stainless steel. The as-deposited films withstand electric fields of 900 kV/cm and exhibit promising room-temperature energy-storage properties: the recoverable energy density reached 7.0 J/cm^3 with an energy-storage efficiency of ∼70%. A post-deposition stress relaxation by annealing at 500 °C further improved the recoverable energy density, leading to 9.8 J/cm^3 with an efficiency of ∼80% [Figure 4]. The energy-storage performance exhibited excellent temperature stability up to 200 °C and electric-field cycling stability up to 16 million cycles.

In collaboration with the Laboratory for Refrigeration and District Energy, the Faculty of Mechanical Engineering, University of Ljubljana we prepared multilayer composites using the aerosol-deposition method. The composite was made of Al_2O_3/Al/Al_2O_3 layers on a magnetocaloric gadolinium substrate. Such ceramic-metal multilayers represent a simple, reliable, and cost-effective approach to functionalizing and protecting existing magnetocaloric substrates and provide an excellent starting point for the development of future electrowetting-on-dielectric devices.

We progressed the research on the **cold sintering** of functional oxides in our **ULTRACOOL** laboratory, expanding the sintering from $BiFeO_3$ ceramics to (K,Na)NbO_3 perovskites and composites with piezoelectric polymers (PVDF). While the optimization of all parameters for the successful cold sintering of the ceramic compounds is still an ongoing process, the first measured electromechanical properties of the sintered ceramics are very promising and show a great perspective of cold-sintered oxides for actuator and energy-storage applications. Preliminary studies show that the main benefits of the cold sintering of ceramics are, besides the energy savings due to the low-temperature processing, their dielectric breakdown strength that allows high voltages applied to the materials without their disintegration, as well as high dielectric permittivity and low dielectric losses.

A miniature ozone generator in the form of a **monolithic three-dimensional ceramic structure** was fabricated by low-temperature co-fired ceramic (LTCC) technology utilising the principle of electric discharge. A multilayered ceramic structure with dimensions of 63.6 mm × 41.8 mm × 1.3 mm included integrated electrodes, buried channels and cavities in micro and millimetre scales. The highest ozone concentration in the LTCC-based ceramic device was around 1.1 vol. % at a voltage of about 7 kV and an oxygen flow rate of 10 ml/min. Its yield is comparable to much larger ozone generators available on the market. The LTCC technology was also implemented to fabricate a 3D structure with a buried cavity for the radio-frequency dielectric heating of polar liquids. The power used to heat water in the cavity with the volume of 0.3 mL ranges from 5 to 40 W. This novel application of dielectric heating could enable the miniaturisation of microfluidic systems. Furthermore, LTCC and high-temperature cofired ceramic (HTCC) materials were tested to fabricate three-dimensional power modules. A dual-pulse electrical test of the power modules confirmed, the quality of metallization, wire bonding, and assembly in combination with selected materials. The research was conducted in collaboration with the company KEKO Equipment and Centre of Excellence NAMASTE.

As part of the **KET4CP** project "Manufacturing of invisible interconnections from solutions of low-cost transparent conduction oxides by screen printing", with project partners RC eNeM and the Institute of Solid State Physics from Latvia, we developed a novel method for fabricating transparent zinc oxide-based thin films on glass from low-cost precursor solutions by chemical solution deposition and screen-printing processes. A high optical transmittance of over 90 % and electrical conductivity of 0.002 S/cm were obtained for 150-nm-thick films processed by screen printing. The solution-derived screen-printing process was successfully demonstrated in the large-scale production line of the company RC eNeM. The Slovenian project partners were awarded the Silver Recognition of the Zasavje Regional Chamber of Commerce in 2021 for the invention.

In collaboration with the Condensed Matter Physics Department, JSI, we studied the memory effect in polydomain liquid-crystal elastomer particles dispersed in a polymer. We confirmed the applicability of flow-induced shear stress in the alignment and deformation of liquid crystal elastomer microparticles in a viscous resin by analysing the rheological behaviour of the composite in terms of temperature and shear-rate-induced changes.

In collaboration with the Condensed Matter Department, JSI, and colleagues from Morocco and France, we investigated lead-free piezoelectric composites for energy harvesting. The composites consist of $Ba_{0.85}Ca_{0.15}Zr_{0.10}Ti_{0.90}O_3$ nanoparticles embedded in a biodegradable polymer. The piezoelectricity and ferroelectricity of the nanoparticles before and after embedding in the polymer matrix were determined by PFM. The maximum power density achieved in the prepared samples was 7.5 mW/cm^3.

In collaboration with the Slovenian company Lotrič Metrology d.o.o., we developed an economical process for producing a non-biological fluid for testing protective medical equipment according to EN 14683 in accordance with ISO 22609: 2004. The technical improvement "Process of preparing a fluid for testing medical protective equipment" was registered.

Some outstanding publications in the past year

1. Kuščer, Danjela, Drnovšek, Silvo, Levassort, Franck. Inkjet-printing-derived lead-zirconate-titanate-based thick films for printed electronics. Materials & design. 2021, vol. 198, str. 109324-1-109324-9. ISSN 0264-1275. DOI: 10.1016/j.matdes.2020.109324. [COBISS.SI-ID 36937475]

2. Benčan, Andreja, Oveisi, Emad, Hashemizadeh, Sina, Veerapandiyan, Vignaswaran K., Hoshina, Takuya, Rojac, Tadej, Deluca, Marco, Dražić, Goran, Damjanović, Dragan. Atomic scale symmetry and polar nanoclusters in the paraelectric phase of ferroelectric materials. *Nature communications*. 2021, vol. 12, no. 1, str. 3509-1-3509-9, ilustr. ISSN 2041-1723. https://www.nature.com/articles/s41467-021-23600-3, DOI: 10.1038/s41467-021-23600-3. [COBISS.SI-ID 65810179]

3. Bradeško, Andraž, Fulanović, Lovro, Vrabelj, Marko, Matavž, Aleksander, Otoničar, Mojca, Koruza, Jurij, Malič, Barbara, Rojac, Tadej. Multifunctional cantilevers as working elements in solid-state cooling devices. *Actuators*. [Online ed.]. 2021, vol. 10, no. 3, str. 58-1-58-13. ISSN 2076-0825. DOI: 10.3390/act10030058. [COBISS.SI-ID 55105027]

4. Šadl, Matej, Condurache, Oana, Benčan, Andreja, Dragomir, Mirela, Prah, Uroš, Malič, Barbara, Deluca, Marco, Eckstein, Udo, Hausmann, Daniel, Khansur, Neamul Hayet, Webber, Kyle Grant, Uršič, Hana. Energy-storage-efficient $0.9Pb(Mg_{1/3}Nb_{2/3})O_3-0.1PbTiO_3$ thick films integrated directly onto stainless steel. Acta materialia, ISSN 1359-6454. [Print ed.], Dec. 2021, vol. 221, str. 117403-1-117403-11, ilustr., doi: 10.1016/j.actamat.2021.117403. [COBISS.SI-ID 81773059]

5. Otoničar, Mojca, Bradeško, Andraž, Salmanov, Samir, Chung, C. C., Jones, Jacob L., Rojac, Tadej. Effects of poling on the electrical and electromechanical response of PMN-PT relaxor ferroelectric ceramics. Open ceramics. 2021, vol. 7, 100140-1-100140-14, ilustr. ISSN 2666-5395. DOI: 10.1016/j.oceram.2021.100140. [COBISS.SI-ID 67640323]

Awards and Appointments

1. Oana-Andreea Condurache: Awarded 3rd place at the Virtual Workshop Contest: YCN Pitch me your Idea!, Young Ceramicst Network Pitch Contest

2. Oana-Andreea Condurache: Awarded 3rd place at the Student Paper Contest, 27th Annual Meeting the Slovenian Chemical Society (SKD 2021)

3. Danjela Kuščer: Silver Award for Innovation: "Manufacture of transparent electrodes from solutions of affordable conductive oxides using screen printing" awarded by Chamber of Comerce Zasavje

4. Andreja Benčan Golob, Goran Dražić, Barbara Malič, Mojca Otoničar, Tadej Rojac, Hana Uršič Nemevšek, Achievement for the paper "Connecting the Multiscale Structure with Macroscopic Response of Relaxor Ferroelectrics" was included in the selection Excellent in science ARRS 2021

5. Matej Šadl: "Alessandro de Vita" award for curiosity and multidisciplinary approach at Crossnano Cross-border Workshop in Nanoscience and Nanotecnology 2021

6. Matej Šadl: Awarded 2nd place at student competition "2021 Joint ISAF ISIF-PMF virtual conference"

Patent granted

1. Vid Bobnar, Barbara Malič, Aleksander Matavž, A method for producing polymeric surface modification layers, SI25887 (A), Slovenian Intellectual Property Office, 31. 03. 2021.

INTERNATIONAL PROJECTS

1. H2020 - ATHENA; Implementing Gender Equality Plans to Unlock Research Potential of RPOs and RFOs in Europe
   Prof. Barbara Malič
   European Commission

2. H2020 - QMatCh; Towards Quantum States of Matter via Chemistry under Extreme Conditions
   Asst. Prof. Mirela Dragomir
   European Commission

3. Cold Sintering of Complex Oxide Materials
   Dr. Mojca Otoničar
   Slovenian Research Agency

4. Low Bandgap Ferroelectric Solar Cell Absorbers: Synthesis and Characterization
   Prof. Hana Uršič Nemevšek
   Slovenian Research Agency

5. Interface Stability of Piezoelectric Ceramic Oxides
   Prof. Tadej Rojac
   Slovenian Research Agency

6. Environmental Benign Sodium Potassium Niobate-based Thick Films for Piezoelectric Energy Harvesting Applications
   Prof. Danjela Kuščer Hrovatin
   Slovenian Research Agency

7. Multiferroics for Solid-State Cooling Applications
   Prof. Hana Uršič Nemevšek
   Slovenian Research Agency

8. Processing – Structure - Properties Study of Environmentally Friendly Piezoelectric Nanoparticles of Tailored Surface Morphology
Prof. Andreja Benčan Golob
Slovenian Research Agency
9. High-Pressure Synthesis and Characterization of Selected Ferroics
Dr. Kristian Radan
Slovenian Research Agency
10. Crystal Growth and Magnetic Properties of Double Perovskites
Asst. Prof. Mirela Dragomir
Slovenian Research Agency
11. Porous Lead-Free Relaxor Ferroelectric Films for Energy Storage
Prof. Hana Uršič Nemevšek
Slovenian Research Agency
12. Environment-Friendly Ferroelectric Oxide Thin Films for Energy Harvesting and Energy Storage Applications
Prof. Barbara Malič
Slovenian Research Agency
13. Realizing In-Situ Studies of Dynamic Mechanisms in Ceramic Oxides in the Reducing Environment in a Transmission Electron Microscope
Prof. Andreja Benčan Golob
Slovenian Research Agency
14. Engineering the Microstructure and Performance of Lead-Free Piezoelectrics for Energy Harvesting
Prof. Barbara Malič
Slovenian Research Agency
15. Environment-Friendly Processing of Lead-Free Functional-Oxide Thin Films for Micro-Electro-Mechanical Systems (MEMS) Applications
Prof. Barbara Malič
Slovenian Research Agency
16. Smart Design of New Multifunctional Composites with Optimized Energy Transfer Across Interfaces between the Components (SoMwOT)
Prof. Barbara Malič
Slovenian Research Agency

RESEARCH PROGRAMME

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

R & D GRANTS AND CONTRACTS

1. In situ atomic level Quantitative Scanning Transmission Electron Microscopy of Functional Materials
Prof. Andreja Benčan Golob
2. TCCbuilder: An open-source simulation tool for thermal control circuits
Prof. Barbara Malič
3. Multicaloric cooling
Prof. Hana Uršič Nemevšek
4. Electrocaloric elements for active cooling of electronic circuits
Prof. Barbara Malič
5. Advanced inorganic and organic thin films with enhanced electrically-induced response
Prof. Barbara Malič
6. The quest for high-temperature superconductvity and exotic magnetism in fluoridoargentates(II)
Asst. Prof. Mirela Dragomir
7. Designing functionality of lead-free ferroelectrics through domain wall engineering
Prof. Andreja Benčan Golob
8. The cool way to polarize
Dr. Mojca Otoničar
9. Engineering of relaxor ferroelectric thin films for piezoelectric and energy storage applications
Prof. Tadej Rojac
10. Structures of elusive noble-gas compounds elucidated by 3D electron diffraction
Asst. Prof. Mirela Dragomir
11. All in One: Multi-caloric and Multi-scavenging Elements for Green Future
Prof. Hana Uršič Nemevšek
12. Enhanced piezoelectricity via structural disorder in polycrystalline relaxor ferroelectrics
Prof. Tadej Rojac
13. MIcrofluidic Sensor System for PESticides detection (MISS PES)
Prof. Danjela Kuščer Hrovatin
14. Flexible elements with multi-physical properties
Prof. Hana Uršič Nemevšek
15. Process intensification for the continuous synthesis of high purity hydrogen peroxide using a micro-scale electrocatalytic reactor
Prof. Barbara Malič

VISITORS FROM ABROAD

1. Maria Karypidou, Aristotle University of Thessaloniki, Thessaloniki, Greece, July 2–August 29, 2021
2. Maximilian Gehringer, Technische Universität Darmstadt, Darmstadt, Germany, September 1 – October 29, 2021
3. Reham Elsurhafa, University of Ankara, Ankara, Turkey, September 13–November 24, 2021
4. Matthieu Fricaudet, Universite Paris-Saclay, Paris, France, October 22 – 29, 2021
5. Maxime Vallet, Universite Paris-Saclay, Paris, France, November 25 – December 4, 2021
6. Prof. Brahim Dkhil, Centrale Supélec, Université Paris-Saclay, Paris, France, December 19 – 21, 2019

STAFF

Researchers
1. Prof. Andreja Benčan Golob
2. Dr. Mirela Dragomir
3. Prof. Goran Dražić*
4. Prof. Danjela Kuščer Hrovatin
5. Dr. Kostja Makarovič*
6. **Prof. Barbara Malič, Head**
7. Dr. Mojca Otoničar
8. Prof. Tadej Rojac
9. Prof. Hana Uršič Nemevšek
Postdoctoral associates
10. *Dr. Uroš Prah, on leave since 15.06.21*
11. *Dr. Kristian Radan, 01.02.21, transferred to Department K1*
Postgraduates
12. Matic Belak Vivod, B. Sc.
13. Oana Andreea Condurache, M. Sc.

14. Sabi William Konsago, M. Sc.
15. Barbara Repič, B. Sc.
16. Samir Salmanov, M. Sc.
17. Matej Šadl, B. Sc.
18. Lia Šibav, B. Sc.
19. Katarina Žiberna, B. Sc.
Technical officers
20. Silvo Drnovšek, B. Sc.
21. Brigita Kmet, B. Sc.
22. Maja Koblar, B. Sc.
Technical and administrative staff
23. Andrej Debevec
24. Tina Ručigaj Korošec, B. Sc.

Note:
* part-time JSI member

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DEPARTMENT FOR NANOSTRUCTURED MATERIALS K-7

The research and development at the Department for Nanostructured Materials are focused on the leading-edge areas of nanotechnology and advanced materials, addressing the most difficult societal challenges that Europe and the world are currently facing. This includes clean and efficient energy, health, environment remediation and critical-raw-materials resource efficiency. A versatile team with synergies across a variety of complementary basic and applied expertise in combination with state-of-the-art research methods enables us to respond promptly to various emerging societal challenges. The basic and applied research of the Department for Nanostructured Materials includes permanent magnets and intermetallic alloys, engineering and functional ceramics, minerals, sensors, materials for a sustainable and ecologically built environment, biomimetic materials and biomaterials.

Head:
Prof. Sašo Šturm

Magnetic materials

We address one of the Europe's Grand Societal Challenges, aligned with the European Green Deal: to make mobility and energy production climate neutral, resource efficient and environmentally friendly, while better closing material loops and avoiding critical-raw-materials dependency. The rare-earth-element-based permanent magnets, like Nd-Fe-B, have the highest maximum energy product $(BH)_{max}$. As such, they are in very high demand for critical applications in electric mobility (e-vehicles), traction and energy-conversion motors, and wind turbines. Through research, we bring new knowledge to the areas of design and production of new, resource-efficient Nd-Fe-B magnets with improved magnetic properties.

Nd-Fe-B permanent magnets typically contain 28–35 wt.% of rare-earth elements (REEs, e.g., Pr, Nd, Tb and Dy). This means that end-of-life (EoL) magnets are an important secondary resource for REEs that the EU considers as the most critical. Upon that, developing efficient recycling methods is one of the EU's top priorities. We have developed a process for recycling Nd-Fe-B PMs via extracting magnetic grains. The method was developed in the frame of an ITN-MSCA project and an EU patent was granted for "A method for recovery of $Nd_2Fe_{14}B$ grains from bulk sintered Nd-Fe-B magnets and/or magnet scraps by electrochemical etching", EP3660174B1 (Figure 1). Currently, the pilot for an upscaled version is set up, being tested and, in parallel, methods based on solely chemical treatments of Nd-Fe-B PMs are being studied to compare the recycling output efficiencies, contribute new findings and advance the Green Deal.

Furthermore, we were awarded a silver medal at the ARCA International Exhibition of Inventions in Zagreb, Croatia, for the innovation "Environmentally friendly and energy efficient method for recovery of rare-earth elements", which provides the complete electrochemical recycling of the rare earths from Nd-Fe-B permanent magnets and contributes to a more sustainable and greener EU future with regards to the recycling of critical raw materials.

We developed a new type of a high-coercivity, nanostructured, Nd-Fe-B-type sintered magnet with graded magnetic properties. A modern technique called Pulsed Electric Current Sintering (PECS) was used to co-sinter powders with different magnetic properties, while simultaneously avoiding diffusion of the elements across the interface between the powders. The results were published in the *Journal of Magnetism and Magnetic Materials* (doi.org/10.1016/j.jmmm.2021.168011).

 A new processing strategy for reusing heavily oxidized scrap Nd-Fe-B magnets was developed. The reprocessing route is based on the PECS of oxidized powders with an addition of Nd-Cu eutectic alloys. With this approach, new permanent magnets with an intrinsic coercivity exceeding 1000 kA/m can be manufactured without using expensive and environmentally hazardous pyro- and hydrometallurgical approaches, and it was officially presented in a master's thesis.
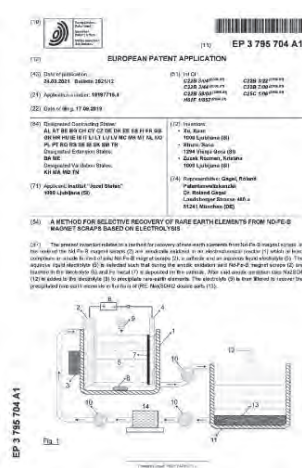
Figure 1: EU PATENT, A method for recovering $Nd_2Fe_{14}B$ grains from bulk sintered Nd-Fe-B magnets and/or magnet scraps by electrochemical etching EP3660174B1 (left); silver medal from the ARCA International Exhibition in Zagreb, Croatia for innovation "Environmentally friendly and energy efficient method for the recovery of rare earth elements", contributing to a more sustainable and greener EU future with regards to the recycling of critical raw materials, i.e., rare earths from permanent magnets (right)

The melt-spun Nd-Fe-B powders were also used for the production of hot-deformed magnets using PECS. The processing conditions were optimized in order to consume a minimal amount of energy and consequently allow cost-effective processing. The results were published in International *Journal of Material Science and Application* (doi.org/10.11648/j.ijmsa.20211005.12). Last but not least, the magnetic properties of the hot-deformed Nd-Fe-B magnets were improved by a recently developed two-step grain-boundary-diffusion method using a minimal amount of heavy rare-earth elements. The corresponding paper was published in *Scripta Materialia (IF = 5.6,* doi.org/10.1016/j.scriptamat.2021.114207 *)*.

In 2021 we continued with the European project SUSMAGPRO, which stands for Sustainable Recovery, Reprocessing and Reuse of Rare Earth Magnets in a European Circular Economy.

The project aims to develop a recycling supply chain for rare-earth magnets in the European Union and demonstrate the effective reuse of recycled rare-earth materials within several industries. The multidisciplinary SUSMAGPRO consortium is composed of 20 of Europe's industry and academic leaders dealing with REEs, focusing on sustainable processing, reuse, recycling, recovery schemes, and covering the whole value chain from the collectors of magnet-containing scrap to the producers of high-tech products.

Another project strongly linked to SUSMAGPRO is INSPIRES (INtelligent and Sustainable Processing of Innovative Rare-Earth magnetS) under the frame of EIT RawMaterials, which started in 2021 and aims to recover and supply rare earths within the EU through radical innovations in the recycling of permanent magnets, focusing on one of the most readily available sources: home appliances. The whole chain of industrial partners in INSPIRES is based in Slovenia and focuses on home appliances that are not involved in SUSMAGPRO. INSPIRES will optimize methods on an industrial scale for the sustainable extraction, recycling and use of recycled magnets in new motors produced in Slovenia. This project will be a proof of concept for a broader European recycling chain of EoL magnets from home appliances.

We successfully coordinated the European project MaXycle (a novel circular economy for sustainable REE-based magnets), a transnational collaborative research and innovation project funded by the ERA-NET Cofund on Raw Materials (ERA-MIN 2) instrument under Horizon 2020. The two most important outcomes from MaXycle are: a) the definition of standardized quality criteria for end-of-life magnets (EOLM) and a classification system for contamination levels, categorizing products by pre-processing requirements, and b) development of a labelling system for newly produced REE magnets to identify different magnet types and qualities, including the provision of reliable and durable marking methods. The project results were published in the journal *Materials Proceedings*, 2021 (doi. org/10.3390/materproc2021005087), and within the "EU Green Week 2021 - ZERO POLUTION."

Since 2021 we have been a member of the H2020–PILOTS PASSENGER project: Pilot Action for Securing a Sustainable European Next Generation of Efficient RE-free magnets; the project proposes improved strontium ferrite (Sr-ferrite) and a manganese-aluminum-carbon (MnAlC) alloys as a substitute to guarantee a sustainable production of permanent magnets in Europe, and we contribute to the Sr-ferrite magnets improvement and characterization.

In 2021 we received funds from the EIT RAW materials network, for the RECO2MAG project, which focuses on the optimization of manufactured permanent magnet microstructures via novel grain-boundary processing to produce resource-efficient sintered NdFeB PMs with a lowered Dy content and improved energy products to be applied in novel e-motors. The LCA/LCC analysis coupled with the latest geological information about critical raw materials will create an independent and efficient EU industry ecosystem.

Within the research project with Kolektor d.d., Slovenian producer of bonded magnets based on Nd-Fe-B, we have improved the coercivity of melt-spun powders used for bonded magnets via the grain-boundary-diffusion process using $Nd_{70}Cu_{30}$ eutectic alloy to process polymer-bonded magnets.

From these results, a patent application entitled "A process for improving the magnetic properties of MQP-B + Nd-Fe-B magnetic powders with a low intergranular phase content and a process for making polymer-bonded magnets from these magnetic powders" has been filed at the Slovenian Intellectual Property Office.

We finished work within the ARRS national project *Effective recycling of abrasive sludge in the production of Sm_2Co_{17} magnets for a waste-free economy* in collaboration with the company Magneti Ljubljana where we are investigating novel recycling of magnetic swarf based on Sm-Co alloys including $SmCo_5$ and Sm_2Co_{17}. We found that magnetic swarf can be recycled with chemical and pyrolytic methods. Afterwards the cleaned swarf can be recycled by applying induction and arc re-melting technologies.

Additive-manufacturing technologies make it possible to produce magnets of arbitrary shapes and magnetization distributions. In order to design a
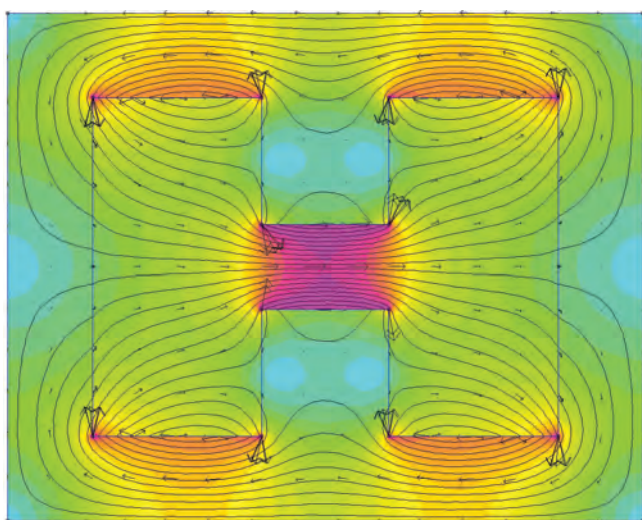
Figure 2: Calculated magnetization profile (red) for a Halbach cylinder, with a homogenous magnetic field inside. A comparison between the prescribed (blue) and calculated (green) pattern.

magnet as the source of a given magnetic-flux field, expressed in terms of the line-of-force pattern, it is necessary to solve the so-called magnetostatic inverse problem. For this purpose, we applied the adjoint-state and finite-element methods. In addition, we proposed the optimum geometry of a permanent magnet as the source of an oscillating magnetic field in a so-called magnetic harvester – a magnetic-induction-based device for charging batteries of portable electronic equipment, for example, smartphones, without applying any external energy sources (Figure 2).

In the frame of the ARRS project *Development of complex-shape multicomponent permanent magnets with the use of advanced 3D printing technology*, we are continuing our work in developing complex-shape, multicomponent, permanent magnets using additive manufacturing for the company Kolektor d.d. We reached the next goal of the project by producing 3D printed parts with orientated Sr-ferrite magnetic particles inside the print. This was reached by exposing the liquefied filament to an external magnetic field that stayed orientated after solidification. The difference in the orientation can be seen in Figure 3.

In 2021 the research activities in the field of mechanical strengthening of ferrite-based ceramic magnets were continued. Here, our research path is following the successful method of strengthening engineering ceramics using cellulose nanofibers (CNFs) developed in collaboration with the colleagues from Materials Science Institute (CSIC) of Madrid. As the integral part of this research, we are exploring the possibilities of a novel fast sintering technique called sintering by intense thermal radiation (SITR). This innovative fabrication of sintered ferrites could replace some of the costly REE-based magnets of lower grades.

This increased the achieved remanence by more than 65%, compared to the 3D print without exposure to an external magnetic field. This will increase the power output of an electric motor using new magnet designs and multi-material usage in a single magnet.

Figure 3: SEM image of the 3D-printed part filled with 60% Sr-ferrite without magnetic alignment (a); with magnetic alignment (b)

Complex intermetallic alloys

In the frame of a collaboration within IRP PAC2, in the field of push-pull alloys based on the Al-Cr-Sc system, we focused on the crystal and electronic structures of a newly discovered ternary phase (Figure 4). The results were published in journal *Crystals (*doi.org/10.3390/cryst11121535*).*

Our main research is focused on the polymer matrix polyphthalamide (PPA) reinforced with Al-Cu-Fe-B quasicrystalline powder. The main objective is the development of low-adhesive high-strength composite materials. PPA belongs to high-temperature engineering plastics and is chemically resistant and ductile. As quasicrystals (QCs) have exciting properties, including low surface energy, low coefficient of friction, high wear resistance, non-stick properties and reduced wetting, the focus of our research was on the surface energy of bulk QCs. The experiments were conducted under ambient conditions mimicking an industrially relevant environment. With X-ray spectroscopy (XPS), we perceived an oxide layer thickness of around 5 nm on the QCs. Oxide can have a unique effect on the bonding of QCs and polymer matrix and, with that, on the composites' surface and mechanical properties, such as high-friction, fretting and cold welding.

Figure 4: (a) Ternary Laves phase viewed in [10$\bar{1}$0] zone axis; (b) density of states; (c) single crystal x-ray diffraction; and (d) Rietveld refinement of newly discovered phase in the Al-Cr-Sc system

Catalysis

Persistent organic pollutants show long-term chemical stability when dispersed in the environment. Examples of such contaminants are pharmaceuticals that can be degraded with the so-called advanced oxidation process (AOP) into their primary constituents, such as carbon dioxide, water and inorganic ions. Within the ongoing study for an ARRS project on the degradation of pharmaceuticals, we successfully evaluated TiO_2, TiON and BDD (boron-doped diamond) materials to degrade antibiotic tetracycline. Within the scope of the research, a review article regarding the photocatalytic, electrocatalytic and photoelectrocatalytic degradation of pharmaceuticals in aqueous media was accepted by the *Journal of Cleaner Production (IF=9.297,* doi.org/10.1016/j.jclepro.2022.131061*).* Moreover, an advanced 3D cell made with additive manufacturing was prepared to reach the final goal: designing efficient flow photoelectrocatalytic reactors for degrading pharmaceuticals in wastewater.

The acquired knowledge on the catalysis of catalytic materials has been successfully implemented within the new framework of researching high-entropy alloys (HEAs). The final goal of the ongoing study is to widen the research of novel materials that could be used for the wastewater treatment of organic pollutants (*e.g., pharmaceuticals*).

We continued our previous collaboration with the National Institute of Chemistry, where TiO_2 nanotubes were prepared with anodic oxidation and treated in ammonia at elevated temperatures. After TiOxNy was formed, Ir

Figure 5: Front cover presenting the manuscript *Toward a Flexible and Efficient TiO₂ Photocatalyst (doi:10.1021/acsomega.1c02862), published in ACS Omega*

nanoparticles were applied to the surface to investigate the effectiveness of the energy-related catalytic reactions.

Next, our successful collaboration with the National Institute of Chemistry also resulted in a patent application at the European Patent Office, Application EP 21163572.7. The topic of the patent is the anodic oxidation of very small metal grids (*e.g., a TEM grid*) and an anodization apparatus that could be applied in a variety of industrial applications.

As part of last year's study research on the anodization of flexible titanium foils in the field of photocatalysis, an article was published in *ACS Omega (IF = 3.512,* doi:10.1021/acsomega.1c02862*)*. The research was featured as the front cover of the ACS journal (Figure 5).

Sensors

We develop receptor elements for detecting various toxic organic components (TOC) and biomolecules such as the SARS-CoV-2 virus. In the field of SARS-CoV-2 detection, we have developed a new type of testing strategy based on electrochemical biosensing for rapid and specific detection of viral variants in saliva samples. The detection system, i.e., a SARS-CoV-2 detection platform, is based on modified screen-printed electrodes (SPEs), enabling the immobilization of various viral receptor elements (antibodies) that are specific to viral variants. Special emphasis has been given to the preparation of modified SPEs, which were constructed of a highly conductive material based on a polystyrene/polyaniline-Au (PS/PANI-Au) nanocomposite. Such a construction is able to translate the specific covalent interaction between antibodies and the corresponding binding viral target into a measurable, concentration-dependent electrochemical signal. After the creation of electrochemical readouts, these data enable a qualitative and quantitative analysis. Also, the fabricated PS/PANI-Au NP composite can exploit its outstanding conductivity and biocompatibility, thus resulting in high analytical sensitivity, specificity and low detection limits (i.e., at attomolar concentration levels). The proposed feasible design of the biosensor platform represents an excellent starting point for the practical and low-cost testing of asymptomatic patients or individuals before symptom onset.

We continued to study the PANI behavior due to the presence of ammonia (NH_3). NH_3 is a part of the natural nitrogen cycle and a toxic, neurotoxic compound indicating a disease state in the human body. Therefore, detecting and monitoring NH_3 concentrations in physiological fluids represent a field of high scientific interest. Electrochemically synthesized PANI is studied for aqueous NH_3 detection at a neutral pH. The sensing system is based on chrono-amperometric measurements and droplet addition of NH_3 aliquot to the background electrolyte (i.e., PBS). The developed sensing mechanism is based on the experimental set-up conditions and results.

The calculated detection limit for the NH_3 detection in phosphate-buffered saline on the PANI electrode (25 μM) was lowered three times by introducing Au nanoparticles on the PANI surface (8 μM). The recovery of PANI after each aliquot addition and the reversibility of measurements indicate further potential application in a flow injection system.

Volatile toxic organic compounds, namely catechol, resorcinol and hydroquinone, are isomers of benzenediols, which gained notoriety of late due to the acute and chronic problems they pose to living beings. These are electrochemically active molecules, meaning they are subject to redox processes. Detection can be performed using a simple three-electrode electrochemical sensor element, wherein the working electrode is made of a material with high conductivity and a large active surface area. This is achieved using a standard SPE, modifying the working electrode by applying a thin layer of carbon-supported catalyst such as Pt/C or Au/C. These modified SPEs were then subjected to cyclic voltammetry for the qualitative detection of single isomers, differential pulse voltammetry for the qualitative detection of multiple isomers in the same analyte, and chronoamperometry for the quantitative detection of single isomers, all in acidic media to boost the electrical conductance of the electrolyte.

The modified SPEs detected three isomers selectively, reaching a detection limit of 1 μM for catechol and hydroquinone, and 100 nM for resorcinol with good reproducibility in laboratory conditions. Our future goals are to improve the detection limits even further, lower the rise times and modify the system for detecting gaseous analytes.
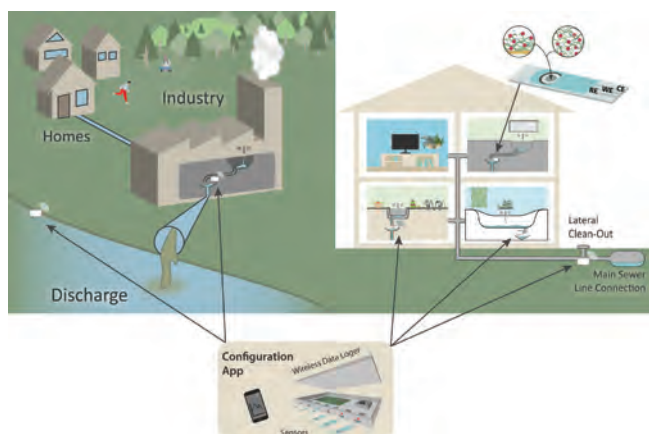
Figure 6: Detection points and working principle of sensor platforms and integration for detection of, e.g., TOCs or PMCs in water

We are developing receptor elements for the detection of toxic organic compounds such as acrylamide (AA) (national project J2-1739), persistent and mobile chemicals (PMCs) (national project J2-3051) and benzenediols. We also developed the receptor element for electrochemical detection of SARS-CoV-2 (national project Z2-3206).

A new area of research is focused on the development of receptor elements for a selective and sensitive detection of persistent and mobile chemicals (PMCs), namely melamine, benzotriazole and BPS (bisphenol S). The sensor development paves the way to a portable and miniaturized sensor able to detect an analyte in water and, in the future, also in air (Figure 6).

Materials for health and a clean environment

We are developing nanocarriers for innovative cancer treatments and diagnostics. In collaboration with Queen's University Belfast, United Kingdom, and the Medical Faculty of the University of Ljubljana, we developed temperature-sensitive liposomes for prostate-cancer treatment containing a prodrug consisting of doxorubicin (Dox) conjugated to a peptide substrate for a prostate-specific antigen (PSA), which can be cleaved by enzymatically active PSA at the tumor site. As-prepared liposomes combined with hyperthermia significantly inhibited tumor growth and metastasis in mice.

The study was published in *Acta Biomaterialia (IF = 8.947,* doi.org/10.1016/j.actbio.2021.12.019*).* We also developed temperature-sensitive liposomes for immuno- and chemotherapy and magnetic resonance imaging (MRI). Doxorubicin therapeutic efficacy was potentiated in combination with anti-PD1 monoclonal antibodies, resulting in a significant reduction in CT26 tumor growth via immune-cell activation. Our study highlights the potential of combining the PD1 blockade with drug-loaded temperature-sensitive magneto-liposomes, where the latter could facilitate chemo/photothermal therapy and MRI-guided drug delivery (Figure 7). This study was performed in collaboration with the researchers from Queen's University Belfast and the Oncology Institute in Ljubljana and published in the *Journal of Controlled Release (IF = 9.776,* doi.org/10.1016/j.jconrel.2021.03.002*).*

In the field of nanocarriers, we have taken a step forward and moved from synthetic liposomes towards cell-based nanocarriers to reduce the possibility of side effects. Erythrocyte membranes have been used as carriers for MRI contrast agents. In the journal *Magnetochemistry* (doi.org/10.3390/magnetochemistry7040051*),* we described the improvement in the contrast efficiency of iron oxide nanoparticles after encapsulation in erythrocyte membranes in comparison with encapsulation in liposomes or free nanoparticles. Fluorescence imaging can be used as a complementary MRI method. Therefore, we encapsulated two different fluorescent dyes (indocyanine green and IR820) in erythrocyte membranes and liposomes, and compared their photothermal efficacy, stability and chemotoxicity with free dyes (published in the *International Journal of Molecular Sciences, IF = 5,924,* doi.org/10.3390/ijms22136914). Finally, we also published a review article on nucleic acid delivery with erythrocyte membrane-based carriers (*International Journal of Molecular Sciences,* doi.org/10.3390/ijms22105264).

Figure 7: PD1 blockade potentiates the therapeutic efficacy of photothermally activated and MRI-guided low-temperature-sensitive magneto-liposomes

Engineering Ceramics

We systematically investigated the dispersion, rheological behavior and freeze casting of aqueous suspensions containing mesoporous alumina (MA) powder. The aim was to prepare stable suspensions containing AlN-hydrolysis-derived, micron-sized particles of γ–Al_2O_3 suitable for consolidation. The addition of divalent cations (Mg^{2+} in Ca^{2+}) or cellulose nanofibers triggered the formation of weak interparticle associations contributing to suspension stabilization. The suspensions were then freeze cast into highly porous MA ceramic monoliths with high hierarchical porosity (93.1–99.2 %) (Figure 8), exhibiting high permeability (k1 = 2.39–4.31×10^{-12} m^2 and k2 = 2.23–9.15×10^{-7} m^2) and low anisotropic thermal conductivity, ranging from 0.039 W/m·K to 0.071 W/m·K that depended on the pore orientation. Despite their high porosity, monoliths displayed remarkably high compressive strengths (up to 52.0 kPa). The work on monoliths was published in *Open Ceramics (* doi.org/10.1016/j.jeurceramsoc.2020.09.014*).*

We focused on the resource effectiveness in ceramics manufacturing to optimize the consumption of commercial alumina during industrial manufacturing of alumina ceramics or different kinds of process losses in terms of generated scraps. We explore the prospects of applying Box-Behnken design

Figure 8: μ–CT imaging of highly porous MA ceramic monoliths viewed in various directions, showing hierarchically columnar meso / macro porosity: a) radial direction, b) 3D view, c) axial direction

by varying the amount of waste alumina scraps and sintering conditions, i.e., comparing the conventional sintering in air and spark-plasma sintering (SPS). The SPS technique enabled rapid densification of alumina compacts in short times, resulting in fine microstructures reflected in higher hardness. The studies were published in the

In the field of dental ceramics, we have been traditionally involved in the interdisciplinary research on zirconia (3Y-TZP) ceramics in collaboration with Department for Prosthetic Dentistry, Medical Faculty, University of Ljubljana (MF-UL). In 2021, at the event *Excellent scientists 2021,* a clinical study of the ageing of 3Y-TZP dental ceramics in the oral environment was selected in the field of Biotechnology and Medicine (Stomatology subfield) among other most prominent research achievements of the past year, chosen by the Slovenian Research Agency (ARRS). The work was published in the leading scientific journal from the field *Dental Materials (*doi.org/10.1016/j.dental.2020.11.023). The study represents an important milestone in the field of research of dental ceramic materials and translational dental medicine (Figure 9).
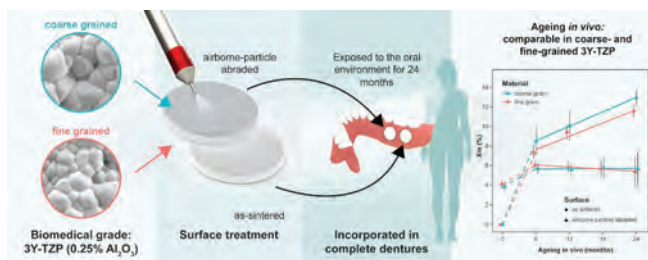
Figure 9: In-vivo aging of zirconia dental ceramics

Building upon a fruitful collaboration with the Faculty of Health Sciences at the University of Ljubljana, we evaluated the extent of bacterial adhesion (*S. mutans*) on four dental materials: two glass–ionomer cements and two ceramic composites. We showed that the highest bacterial adhesion was on the nano-hybrid composite surface, which, in this study, was associated with the lowest contact angle, highest roughness and the most negative zeta potential. The results were published in *Coatings (*doi.org/10.3390/coatings11020235*). S. mutas* has also been evaluated against a broader range of dental materials, from amalgam, Chromasit, YSZ and a removed tooth. The adhesion was the highest (by a significant amount) on the tooth, followed by YSZ ceramics. The lowest adhesion was observed on amalgam. The study was published in *Molecules (*doi.org/10.3390/molecules26041152*).*

Moreover, bacterial adhesion on prosthetic and orthotic parts was investigated. The adhesion of *S. aureus and S. epidermis* (causing severe infection at the material-skin junction) was evaluated against natural and artificial cork, leather, foams, PMMA and PVA.

The highest adhesion was observed on synthetic leather and thermo cork – both materials exhibit diverse and complex surface morphologies that protect against lateral forces and increase biofilm formations. The results were published in two studies: in *Coatings (*doi.org/10.3390/coatings11121469*) and Materials (*doi.org/10.3390/ma14226877*).*

Finally, we studied the effect of polyelectrolyte multilayer coatings (positively and negatively terminated layers) on urinary catheter surfaces against the *E. coli* adhesion. An analysis of the properties of the uncoated and coated surfaces revealed that the most significant difference is related to the charge (i.e., zeta potential) of the examined surfaces, while the roughness and hydrophobicity of the examined surfaces are similar. The study was published in *Coatings (*doi.org/10.3390/coatings11060630*).*

Figure 10: W-11WC monoblock joint with a CuCrZr tube (left); the same mock-up exposed to a thermal shock of 15 MW/m² while being cooled with a cooling liquid (at a temperature of 18 °C (right)

As part of the structural materials research, K7 researchers were awarded with a new project under the European fusion program EUROfusion for the period 2021–2025. During this period, we will have continued our research in the field of W-W$_2$C composites with various compositions, also using additive manufacturing of functionally graded materials (such as Cu-W).

The composition and preparation process of W-W$_2$C composite materials were optimized based on the study of interdependent relationships between the initial and final compositions of the material, which directly affect its temperature-dependent (up to 1000 °C) mechanical and thermal properties. The main criterion for selecting the optimal composition was the resistance of the material to thermal shocks during a high-heat-flux test (HHFT). Based on the promising thermomechanical properties and HHFT, determined in the previous period, the W-11WC composition (Figure 10) was selected for the production of test monoblocks for the divertor. The composite monoblocks were joined with a CuCrZr cooling tube and subjected to HHFTs in an actively cooled divertor model.

By changing the W-W$_2$C ratio of the composites, we also prepared a W-W$_2$C composite whose brittle-ductile transition temperature is as much as 200 °C lower than that of the currently most promising and investigated material – rolled tungsten.

Biomaterials

In 2021 the biomaterials research on titanium implants conducted in previous years was granted a European patent "Implant having a multilayered coating and a process for preparing thereof" (EP2595669A1). The patent describes the invention related to the creation of a hydrothermally prepared titania coating and a particulate

sol-gel bioactive glass coating on a porous titanium-based implant to improve the implant integration with bone. As a partner in an ARRS-funded project, being carried out in collaboration with the Faculty of Veterinary Medicine, University of Ljubljana, in 2021 we completed our research on the silk fibroin carrier for hormone release. This study was published in the leading scientific journal in the field of drug-delivery science and pharmaceutical technology (*Journal of Drug Delivery Science and Technology,* doi.org/10.1016/j. jddst.2021.102701*).* Preparing biopolymer xerogels is an important step in developing advanced pharmaceutical delivery systems for hormone therapy with prolonged drug release (Figure 11). Further research was focused on the preparation of fibroin films with a low degree of crystallinity to increase the degradation rate of the hormone-releasing implant. The remaining in vivo animal tests were performed.
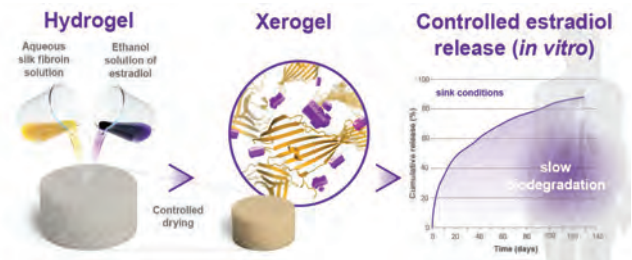
Figure 11: Stages in the development of silk fibroin xerogel delivery systems with prolonged estradiol release

Functional ceramics: semiconducting ZnO-based ceramics (varistors, thermoelectrics)

Thermoelectric ZnO ceramics are relevant for harvesting electricity from waste heat at high temperatures above 650 °C. ZnO is an n-type semiconductor with a high Seebeck coefficient (S) of -400 mV/K. Unfortunately, its electrical conductivity (s) is too low for a good thermoelectric material due to the low concentration of charge carriers where n <10-17cm^{-3}, while its thermal conductivity is too high as it has a simple structure consisting of light elements.

Understanding the influence of dopants on the concentration of charge carriers, and structural and microstructural elements on the transport of charge carriers and phonons is thus crucial for improving electrical conductivity (s) while maintaining a high Seebeck coefficient (S) and reducing thermal conductivity. Our research is thus focused on studying the influence of boundary surfaces such as grain boundaries and specific inverse boundaries (IBs) in grains on the charge and heat transport. In particular, multiple IBs caused by dopants such as In^{3+} and Ga^{3+} play an important role as they can act as an energy filter where phonon and electron pathways split. With its width limited to one layer of atoms and practically infinite in the other two dimensions, an IB can behave like a quantum well, where only electrons of a certain energy are allowed to pass it, while the others remain confined to the layer. At the same time, donor dopants (M^{3+}) can cause a multitude of available states to transport electrons that switch to the ballistic transport mode (s_b) along a planar defect. On the other hand, 2D structural and chemical anisotropy causes the scattering of phonons that transversely pass planar defects, which lowers k across the layer. Accordingly, we analyzed the effects of additions of small amounts of up to a few at. % of dopants such as In^{3+}, Al^{3+} and $Co^{2+,3+}$ on the structure, microstructure and thermoelectric properties of ZnO ceramics in the $ZnO-In_2O_3-Co_3O_4$, $ZnO-Al_2O_3-Co_3O_4$ and $ZnO-In_2O_3-Al_2O_3-Co_3O_4$ systems. In this research we are collaborating with the National Institute for Materials Science (NIMS, Tsukuba, Japan) and the CRISMAT Laboratory (Caen, France).

In collaboration with the Shanghai Institute of Ceramics and Chinese Academy of Science – SICCAS, we studied the influence of selected dopants and process parameters (temperature and sintering atmosphere) on the formation of electrostatic Schottky barriers at grain boundaries and electrical conductivity of ZnO ceramics.

We found that sintering in a reductive atmosphere effectively prevents the formation of intrinsic acceptor states, i.e., zinc vacancies (V_{Zn}) and oxygen interstitials (O_i), and thus Schottky barriers, while also greatly increasing the solid solubility of Al_{3+} in ZnO, which significantly improves electrical conductivity and thermoelectric properties of ZnO ceramics.

These studies also led to the discovery of a completely new type of ZnO-based varistor ceramic, in which the formation of electrostatic Schottky barriers responsible for the current-voltage (I-U) nonlinearity is caused by Cr_2O_3, while additions of small amounts of Ca, Co and Sb oxides furtherly enhance it (published in *ACS Applied Materials & Interfaces*, doi.org/10.1021/acsami.1c07735).

In comparison with the currently known standard varistor ceramics based on ZnO, the new type of the ZnO-Cr_2O_3 varistor ceramics do not contain volatile (Bi_2O_3), expensive (Pr_6O_{11}) and toxic (V_2O_5) dopants, while their advantage is also a simple and significantly cheaper chemical composition. We explained the mechanism of the formation of electrostatic Schottky barriers with the addition of Cr_2O_3 and investigated the influence of a CaO addition on the ZnO grain growth and breakdown voltage, which is important for the possibility of using the new type of varistor ceramics for overvoltage protection in a broad range of voltages (Figure 12).
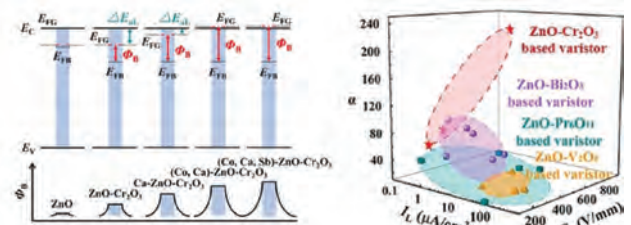
Figure 12: Exceptional current-voltage (I-U) nonlinearity of the novel ZnO-Cr_2O_3-base varistor ceramic is related to the band structure and added performance enhancers (i.e., oxides of Ca, Co and Sb); f_B – Schottky barrier height, E_C – conduction band, E_V – valence band, E_{FB} and E_{FG} – Fermi levels in the grain boundaries and grains (left); nonlinear coefficient (a), leakage current (I_L) and breakdown voltage (E_B) of the novel (Ca,Co,Sb)-doped ZnO-Cr_2O_3-based varistor ceramics compared to the literature data of the standard types of ZnO-based varistor ceramics (right).
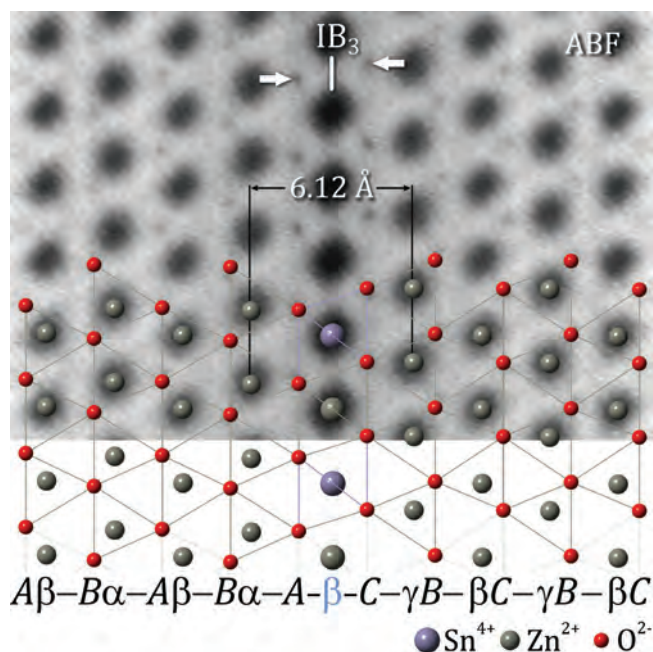
Figure 13: Overlaid DFT relaxed model of Sn-rich IBs (stripe variant of the cation distribution) with a stacking sequence of the IB$_3$ translation (Science of Sintering, doi.org/10.2298/SOS2102237R).

We collaborated with companies Bourns and KEKON in the development of multilayer varistors (MLVs) with improved temperature stability and components based on MLVs and multilayer capacitors. In collaboration with the Faculty of Mechanical Engineering of the University of Ljubljana and company VARSI, we studied the characteristics of surfaces and processing of the surfaces of varistor ceramics to optimize the finalization of varistors and their properties.

A high-resolution ABF-STEM image of Sn-rich IBs in ZnO viewed in the [21-1-0] projection (Figure 13) shows the positions of O-columns (weak dark dots). These help us identify coordination of cations and the type of polarity inversion. Below is an overlaid DFT relaxed model of the Sn-rich IBs (stripe variant of the cation distribution) with a stacking sequence of the IB$_3$ translation (published in *Science of Sintering,* doi.org/10.2298/SOS2102237R).

Inversion boundaries in ZnO were further studied in a SnO$_2$-doped system where the Sn^{4+} dopant forms disordered arrangements with Zn^{2+} in a 1:1 ratio in the octahedral IB layer. The in-plane composition is driven by the local charge balance, following Pauling's principle of electroneutrality for ionic crystals, according to which the average oxidation state of cations in an IB layer is $^{3+}$. Atomic-scale HRTEM and ABF–STEM analyses of the Sn-rich IBs confirmed two short-range in-plane distributions of cations that were first identified by density functional theory (DFT) calculations as the lowest energy cation arrangements. As a result, the cation ordering intermittently changes its type and direction to maximize the intrinsic entropy of the IB layer driven by the in-plane electroneutrality and six-fold symmetry restrictions. A long-range in-plane disorder, as shown by our work, would enhance the quantum well effect on phonon scattering, while Zn^{2+} located at the IB sites modify the bandgap, and enhance the in-plane conductivity and concentration of carriers.

Mineralogy

The collaboration with the Department for Litospheric Research of the Vienna University in the frame of FWF–ARRS bilateral project N1–0115: "Mineral inclusions in garnets from macroscopic to atomic scale – opening the petrogenetic archive (GInA)" and FWF–RFBR international joint project: "Fe–Ti oxide inclusions and magnetism of oceanic gabbro (MiMa)" resulted in a joint publication of *Formation pathways of oriented magnetite micro-inclusions in plagioclase from the oceanic gabbro* that was published in *Contributions to Mineralogy and Petrology (*doi.org/10.1007/s00410-021-01864-8*).* It presents a comprehensive investigation of the magnetite inclusions in plagioclase. Garnets from two Austrian localities were further studied in terms of syngenetic inclusions to explain their growth conditions. A bilateral NKFIH–ARRS project with the University of Pannonia in Veszprém, N1–0230: "Aragonite: Structure and formation" was approved for funding.

The University of Novosibirsk was included as an external partner. The application was based on long-standing expertise of the groups in the field of aragonite formation. Linked to this subject, a study on metastable structures of CaCO$_3$ and their relation to aragonite was jointly published with the Novosibirsk group in *Crystal Growth & Design (*doi/10.1021/acs.cgd.0c00589*).*
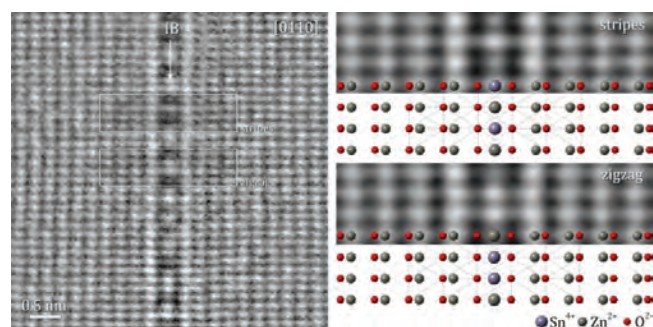
Figure 14: Quantitative HRTEM study of Sn-rich inversion boundaries in ZnO showing two different short-range arrangements of cations in the IB-plane. Cation arrangements (stripes and zigzag) are controlled by the IB chemistry and six-fold in-plane symmetry limitations, Acta Materialia, doi.org/10.1016/j.actamat.2020.08.035).

Advanced electron microscopy

For the microstructural characterization of materials, we use scanning electron microscopy (SEM), transmission electron microscopy (TEM), light optical microscopy (LOM) and atomic force microscopy (AFM). Among SEM techniques we use high-resolution FEGSEM imaging, qualitative and quantitative electron-probe microanalysis (EPMA: EDXS, WDXS) and electron-backscatter diffraction (EBSD). Among TEM techniques high-resolution scanning transmission electron microscopy (STEM, HAADF-STEM), electron-energy-loss spectroscopy (EELS) and EDXS are used for structural and chemical analysis of materials at the atom scale (Figure 14). Recently, in-situ liquid-cell TEM has been employed to observe dynamical processes during electrochemical processes of metal deposition from liquid media.

The ESTEEM consortium (Enabling Science and Technology through European Electron Microscopy) continued its activities within the ESTEEM3 project in the field of materials characterization using state-of-the-art transmission electron microscopy techniques.

The research group of the Department for Nanostructured Materials is strongly connected with the activities within the Center for Electron Microscopy and Microanalysis (CEMM), mainly through the implementation of various electron microscopy analytical techniques and the possibility for the researchers to access the research infrastructure for electron microscopy.

Industrial partners

Our industrial cooperation includes the following companies: Arhel d.o.o. Žeje pri Komendi, Gorenje d.o.o. Velenje, Institute for Water of the Republic of Slovenia, Kekon d.o.o. Žužemberk, Kolektor Group d.o.o. Idrija, Magneti d. d. Ljubljana, RLS Merilna tehnika d.o.o. Žeje pri Komendi, University of Ljubljana – Faculty of Mechanical Engineering, Weiler Abrasives d.o.o. Maribor.

Education and outreach activities

For the ninth year, the members of the department participated in the science-promotion activities within the framework of the Science on the Street project. We organized 16 live and/or virtual popular-science lectures. On the ZnC website, we published 5 blogs by researchers and 2 contests. At the invitation of the EIT "Raw Materials" and JA Slovenia (Institute for the Promotion of Youth Entrepreneurship), we co-organized the Innovation Camp 2021. A total of 137 students from 17 high schools from all over Slovenia participated at the Innovation Camp.

SRIP ToP activities, vertical value chain (VVV) new materials

Within the SRIP ToP VVV New Materials activities, we prepared additions to the accepted Action Plan for the 3rd phase of SRIP ToP for the period 2020–2023, following the successful conclusion of the 2nd phase.

Awards and Appointments

1. Dr Tomaž Tomše is a scholarship recipient for research and for a new approach towards the manufacture of advanced multicomponent Nd-Fe-B permanent magnets for electromotors and and generators. The award is given by the Slovenian Science Foundation (SSF) in cooperation with the World Federation of Scientists (WFS).
2. Prof. Sašo Šturm, Prof. Kristina Žužek, Xuan Xu are recipients of the Silver Medal for Innovation at the ARCA International Exhibition "Enviromentally friendly and energy effecient method for recovery of rare earth elements", awarded by the Croatian Association of Innovators, Zagreb, Croatia.

Organization of conferences, congresses and meetings

1. Closing meeting of the international project MaXycle: A novel circular economy for sustainable RE-based magnets (ERA.MIN2), Goriška Brda, 20–22 June 2021
2. Annual meeting within the international laboratory LIA PACS2: Push-Pull AlloyS and Complex Compounds (PACS2): from bulk properties to surface functions, Goriška Brda, 8–10 November 2021
3. Annual meeting within the international project EIT Raw Materials INSPIRES: Intelligent and Sustainable Processing of Innovative Rare-Earth Magnets, Ribno at Bled, 14–16 December 2021

Patents granted

1. Simon Reinhard, Jaćim Jaćimović, Lorenz Herrmann, Tomaž Tomše, Method of producing a permanent magnet with inter-grain heavy-rare-earth element, EP3649659 (B1), European Patent Office, 07. 04. 2021.
2. Saša Novak, Nataša Drnovšek, Gregor Murn, Implant having a multilayered coating and a process for preparing thereof, EP2595669 (B1), European Patent Office, 13. 10. 2021.
3. Xuan Xu, Sašo Šturm, Kristina Žužek Rožman, A method for recovery of $Nd_2Fe_{14}B$ grains from bulk sintered Nd-Fe-B magnets and/or magnet scraps by electrochemical etching, EP3660174 (B1), European Patent Office, 27. 10. 2021.
4. Sašo Gyergyek, Andraž Kocjan, Darko Makovec, Method for synthesis of coated magnetic particles GB2582272 (B), Intellectual Property Office, 14. 07. 2021.

INTERNATIONAL PROJECTS

1. K7, CTT - ID Creations; Rights and Obligations regarding the Development, Use and Commercialization of Hydrothermally Synthetized TiO2 Coatings in Metal Orthopaedic and Dental Implants
   Prof. Saša Novak Krmpotič
   Id Creations Oy

2. COST CA17140 - Nano2Clinic; Cancer Nanomedicine - From the Bench to the Bedside
   Dr. Nina Kostevšek
   Cost Association Aisbl

3. Stay of Ipeknaz Özden at IKTS, Fraunhofer Institute for Ceramic Technologies and Systems IKTS, Dresden, Germany on Project: Integration of Fused Filament Fabrication with Thermoplastic 3D Printing for Improving Mechanical Performance
Ipeknaz Özden
Jecs Trust

4. H2020 - ESTEEM3; Enabling Science and Technology through European Electron Microscopy
Prof. Miran Čeh
European Commission

5. H2020 - SUSMAGPRO; Sustainable Recovery, Reprocessing and Reuse of Rare-Earth Magnets in a Circular Economy
Prof. Spomenka Kobe
European Commission

6. H2020 - ATHENA; Implementing Gender Equality Plans to Unlock Research Potential of RPOs and RFOs in Europe
Prof. Spomenka Kobe
European Commission

7. H2020 - ORACLE; Novel Routes and Catalysts for Synthesis of Ammonia as Alternative Renewable Fuel
Prof. Andraž Kocjan
European Commission

8. H2020 - PASSENGER; Pilot Action for Securing a Sustainable European Next Generation of Efficient RE-Free Magnets
Prof. Kristina Žužek
European Commission

9. H2020 - EUROfusion; Plasma Facing Components-1-IPH-FU, EUROfusion
Prof. Saša Novak Krmpotič
European Commission

10. Tailoring Thermoelectric Properties through Defects Engineering in ZnO Bulk Ceramics
Prof. Slavko Bernik
Slovenian Research Agency

11. Nanostructured Metal Oxide-Based Materials for Applications in Photocatalytic Processes
Dr. Matejka Podlogar
Slovenian Research Agency

12. INSPIRES - Intelligent and Sustainable Processing of Innovative Rare-Earth Magnets
Prof. Spomenka Kobe
Eit Rawmaterials E.v.

13. HE - EUROfusion; WP18: MAT_HE-FU, IREMEV-MAT-1_HE-FU, IREMEV-MAT-2_HE-FU, IREMEV-MAT-3_HE-FU
Dr. Petra Jenuš
European Commission

14. HE - EUROfusion; WP21: PRD-1,2_HE-FU
Dr. Aljaž Iveković
European Commission

15. HE - EUROfusion; WP24: TRED_HE-FU, EDU_HE-FU
Prof. Saša Novak Krmpotič
European Commission

RESEARCH PROGRAMMES

1. Nanostructured Materials
Prof. Sašo Šturm
2. Ceramics and complementary materials for advanced engineering and biomedical applications
Prof. Andraž Kocjan
3. Fusion technologies
Prof. Saša Novak Krmpotič

R & D GRANTS AND CONTRACTS

1. Role of estrogens in active brain feminisation? and development of a novel hormone implant, mimicking estrous cycle
Prof. Saša Novak Krmpotič
2. Characterization of fractal structures and scale-up parameters in their synthesis
Dr. Matejka Podlogar
3. Development of a new reactor concept for microkinetic studies and its use for selective oxidative dehydrogenation of alkanes and methane coupling
Dr. Luka Suhadolnik
4. Selective extraction of high value molecules from forest products processing residues in the speciality chemicals sector
Dr. Petra Jenuš
5. Molybdenum geobiochemical Cycle in modern environments
Prof. Sašo Šturm
6. Advanced 3D cell models: Bridging the gap between in vitro and vivo experimental systems (hep3DGenTox)
Prof. Saša Novak Krmpotič
7. Post-radiation caries in head and neck cancer patients: Understanding and prevention
Prof. Andraž Kocjan

8. Degradation of plastics with polyextremotolerant fungi
Dr. Matejka Podlogar
9. Modulation of fruit polyphenolic profile by sustainable postharvest physical treatments
Dr. Anže Abram
10. Preclinical and Clinical Investigations of Zirconia Dental Ceramics Fabricated by Additive Manufacturing Technologies (ZIRAMDENT)
Prof. Andraž Kocjan
11. Nanoscale investigations of diffusion controlled topotaxial phase transformations in rutile-corundum host systems
Prof. Aleksander Rečnik
12. Towards reliable implementation of monolithic zirconia dental restorations
Dr. Andraž Kocjan
13. Mineral inclusions in garnet from macroscopic to atomic scale: Opening the petrogenetic archive
Prof. Aleksander Rečnik
14. High performance nanostructured acrylamide sensors
Asst. Prof. Kristina Žagar Soderžnik
15. Designing functionality of lead-free ferroelectrics through domain wall engineering
Asst. Prof. Matej Andrej Komelj
16. Prediction of the initial stages of electrochemical phase formation by multi-scale modelling and insitu transmission electron microscopy
Prof. Sašo Šturm
17. Extended defects in natural and synthesized perovskite oxides: nanogeochemcial indicators and functional interfaces
Prof. Aleksander Rečnik
18. Development of High Performance Sensors for Detection of Persistent and Mobile Chemicals in the Environment (SENSE-PMC)
Asst. Prof. Kristina Žagar Soderžnik
19. Effective recycling of abrasive sludge in the production of Sm2Co17 magnets for a waste-free economy
Prof. Kristina Žužek
20. Development of complex shape multicomponent permanent magnets with the use of advanced 3D printing technology
Prof. Spomenka Kobe
21. Degradation of textile microplastic for domestic wastewater treatment
Dr. Matejka Podlogar
22. Novel Flow Photoelectrocatalytic Reactors for Degradation of Pharmaceuticals in Waste Water
Prof. Miran Čeh
23. RECEMENT:Re-generating (raw) materials and end-of-life products for re-use in Cement/Concrete
Prof. Sašo Šturm
Ministry of Education, Science and Sport
24. A novel ciruclar economy for sustainable RE-based magnets
Prof. Spomenka Kobe
Ministry of Education, Science and Sport
25. Financing of projects visits at the Slovenian higher education institutions
Prof. Sašo Šturm
Public Scholarship, Development, Disability and Maintenance Fund of the Republic of Slovenia
26. Services for the Exports
Dr. Zoran Samardžija
27. External Services
Prof. Andraž Kocjan

NEW CONTRACTS

1. Effective recycling of abrasive sludge in the production of Sm2Co17 magnets for a waste-free economy
Prof. Kristina Žužek
Magneti Ljubljana, d. d.
2. NexGenHVEC: Advanced materials, technologies and prototypes for cost effective hybrid varistor electronic components with improved thermal stability
Prof. Sašo Šturm
Kekon d. o. o.
3. Degradation of textile microplastic for domestic wastewater treatment
Dr. Matejka Podlogar
Gorenje gospodinjski aparati, d.d.
4. Development of complex shape multicomponent permanent magnets with the use of advanced 3D printing technology
Prof. Spomenka Kobe
Kolektor group d. o. o.
5. Measurements on the vibrating sample magnetometer, x-ray diffractometer and transmission electron microscope on the CoNiP system
Prof. Sašo Šturm
Rls merilna tehnika d. o. o.
6. Novel Flow Photoelectrocatalytic Reactors for Degradation of Pharmaceuticals in WasteWater
Prof. Miran Čeh
Arhel projektiranje in inženiring d. o. o.

VISITORS FROM ABROAD

1. Milan Vukšić, University of Zagreb, Faculty of Mechanical Engineering and Naval Architecture (FSB), Zagreb, Croatia, 15–31 January 2021
2. Martina Kocijan, University of Zagreb, Croatia, 1 February–31 March 2021
3. Milan Vukšić, University of Zagreb, Faculty of Mechanical Engineering and Naval
4. Architecture (FSB), Zagreb, Croatia, 1 February–31 March 2021
5. Assoc. Prof. Aleš Omerzu in Asst. Dr Robert Peter, University of Rijeka, Rijeka, Croatia, 2 June 2021
6. Dr Pascal Boulet, Thiago Trevizam Dorini, dr Emilie Gaudry, dr Julian Ledieu in Marie-Cécile de Weerd, Jean Lamour Institute – University of Lorraine, Nancy, France, 7–11 June 2021
7. Dr Vincent Fournee, Jean Lamour Institute – University of Lorraine, Nancy, France, 22–25 June 2021
8. Anna Katharina Hofer, Chair for Structure and Functional Ceramics, Montanuniversität Leoben, Austria 6–9 July 2021
9. Daria Jardas, University of Rijeka, Rijeka, Croatia, 13–24 July 2021
10. Dr Florian Brix in dr Emilie Gaudry, Jean Lamour Institute – University of Lorraine, Nancy, France 2–6 August 2021
11. Thiago Trevizam Dorini, Jean Lamour Institute – University of Lorraine, Nancy, France, 2–12 August 2021
12. Sandra González Arceo, Autonomous University of Madrid International Relations and Mobility Service, Madrid, Spain, 13 September 2021–31 January 2022
13. Dr Richard Wheeler, Edinburgh Scientific, Edinburgh, United Kingdom, 16 September 2021
14. Darya Farrokhnemou and SeyyedehShahrzad Sajjadivand, Faculty of Engineering and Natural Sciences, Sabancı University, Istanbul, Turkey, 16 September–13 December 2021
15. Assoc. Prof. Aleš Omerzu, University of Rijeka, Rijeka, Croatia, 27 September–27 December 2021
16. Krzysztof Kubacki, Innovation Center for the Eastern Region of the Republic of Slovenia and Tina Zajc Benda, EIT RawMaterials Innovation Hub CLC East Sp. z o. o, Wroclaw, Poland, 14 October 2021
17. Dr Gabin Guélou, prof. dr Emmanuel Guilmeau in Krishnendu Maji, CRISMAT laboratory, Caen, France, 26–29 October 2021
18. Anna Katharina Hofer, Chair for Structure and Functional Ceramics, Montanuniversität Leoben, Austria, 8–12 November 2021
19. Anna Katharina Hofer, Chair for Structure and Functional Ceramics, Montanuniversität Leoben, Austria, 13–15 December 2021
20. Dr Goran Branković in Jelena Vukašinović, Institute for Multidisciplinary Research (IMSI), Belgrade, Serbia, 13–16 December 2021
21. Prof. Carlo Burkhardt, Pforzheim University - University of Applied Sciences with the faculties of design, technology and economics and law, Pforzheim, Germany, 16–18 December 2021

STAFF

Researchers
1. Prof. Slavko Bernik
2. Prof. Miran Čeh
3. Prof. Jean Marie Dubois
4. Dr. Aljaž Iveković
5. Dr. Petra Jenuš
6. Prof. Spomenka Kobe
7. Prof. Andraž Kocjan
8. Asst. Prof. Matej Andrej Komelj
9. Prof. Saša Novak Krmpotič
10. Dr. Matejka Podlogar
11. Dr. Benjamin Podmiljšak
12. Prof. Aleksander Rečnik
13. Dr. Zoran Samardžija
14. **Prof. Sašo Šturm, Head**
15. Dr. Kristina Žagar Soderžnik
16. Prof. Kristina Žužek

Postdoctoral associates
17. Dr. Anže Abram
18. Dr. Belisa Alcantara Marinho
19. Dr. Maja Antanasova*
20. Dr. Nataša Drnovšek*
21. *Dr. Andrea Impagnatiello, left 01.09.21*
22. *Dr. Fevzi Kafexhiu, left 01.09.21*
23. Dr. Sina Khoshsima
24. Dr. Nina Kostevšek
25. Sorour Semsari Parapari, M. Sc.
26. *Dr. Luka Suhadolnik, on leave since 01.10.21*
27. Dr. Tomaž Tomše
28. Dr. Špela Trafela

Postgraduates
29. Giulia Della Pelle, M. Sc.
30. *Hermina Hudelja, B. Sc., left 15.03.21*
31. Diana Knyzhnykova, M. Sc.
32. Matej Kocen, B. Sc.
33. Dr. Matic Korent
34. Anja Korent, B. Sc.
35. Abhilash Krishnamurthy, M. Sc.
36. Monika Kušter, B. Sc.
37. Barbara Ljubec, B. Sc.
38. Živa Marinko, B. Sc.
39. Ipeknaz Özden, M. Sc.
40. Patrick Seleš, M. Sc.
41. Vinko Sršan, M. Sc.
42. *Sara Tominc, B. Sc., left 01.07.21*
43. Aleksander Učakar, B. Sc.
44. Anubhav Vishwakarma, M. Sc.

Technical officers
45. Sanja Fidler, B. Sc.
46. Kaja Križman, B. Sc.
47. Tina Radošević, B. Sc.
48. Dr. Boris Saje*

Technical and administrative staff
49. Sabina Cintauer, B. Sc.
50. Darko Eterović
51. Tomislav Pustotnik
52. Marija Šebjan Pušenjak, B. Sc.

Note:
* part-time JSI member

BIBLIOGRAPHY

ORIGINAL ARTICLE

1. Tian Tian, Liaoying Zheng, Matejka Podlogar, Zeng Huarong, Slavko Bernik, Kunqi Xu, Xuezheng Ruan, Xun Shi, Guorong Li, "Novel ultrahigh-performance ZnO-based varistor ceramics", *ACS applied materials & interfaces*, 2021, **13**, 30, 35924-35929.
2. Leonard Moriau *et al.* (12 authors), "Effect of the morphology of the high-surface-area support on the performance of the oxygen-evolution reaction for iridium nanoparticles", *ACS catalysis*, 2021, **11**, 2, 670-681.
3. Živa Marinko, Luka Suhadolnik, Barbara Šetina, Vid Simon Šelih, Boris Majaron, Janez Kovač, Miran Čeh, "Toward a flexible and efficient TiO$_2$ photocatalyst immobilized on a titanium foil", *ACS omega*, 2021, **6**, 36, 23233-23242.
4. Julian Ledieu, Michael Feuerbacher, Carsten Thomas, Marie-Cécile de Weerd, Sašo Šturm, Matejka Podlogar, Jaafar Ghanbaja, Sylvie Migot, Muriel Sicot, Vincent Fournée, "The (110) and (320) surfaces of a Cantor alloy", *Acta materialia*, 2021, **209**, 116790.
5. Leonard Moriau, Gorazd Koderman Podboršek, Angelja Kjara Surca, Sorour Semsari Parapari, Martin Šala, Urša Petek, Marjan Bele, Primož Jovanovič, Boštjan Genorio, Nejc Hodnik, "Enhancing iridium nanoparticles' oxygen evolution reaction activity and stability by adjusting the coverage of titanium oxynitride flakes on reduced graphene oxide nanoribbons' support", *Advanced materials interfaces*, 2021, **8**, 17, 2100900.
6. Martina Kocijan *et al.* (11 authors), "Graphene-based TiO$_2$ nanocomposite for photocatalytic degradation of dyes in aqueous solution under solar-like radiation", *Applied sciences*, 2021, **11**, 9, 3966.

7. Špela Trafela, Sašo Šturm, Kristina Žužek Rožman, "Surface modification for the enhanced electrocatalytic HCHO oxidation performance of Ni-thin-film-based catalysts", *Applied Surface Science*, 2021, **537**, 147822.

8. Laurent Boulley, Dmytro Kandaskalov, Marie-Cécile de Weerd, Sylvie Migot, Jaafar Ghanbaja, Sašo Šturm, Pascal Boulet, Julian Ledieu, Émilie Gaudry, Vincent Fournée, "Investigation of the (100) and (001) surfaces of the Al_5Fe_2 intermetallic compound", *Applied Surface Science*, 2021, **542**, 148540.

9. Igor Karlovits, Urška Kavčič, Špela Trafela, Kristina Žužek Rožman, "Comparison of cyclic voltammetry measurements of paper-based screen printed electrodes via proprietary and open source potentiostats", *Bioresources*, 2021, **16**, 2, 3916-3933.

10. Martina Kocijan, Lidija Ćurković, Tina Radošević, Matejka Podlogar, "Enhanced photocatalytic activity of hybrid $rGO@TiO_2/CN$ nanocomposite for organic pollutant degradation under solar light irradiation", *Catalysts*, 2021, **11**, 9, 1023.

11. Mia Omerašević, Andraž Kocjan, Dušan Bučevac, "Novel cordierite-acicular mullite composite for diesel particulate filters", *Ceramics international*, 2021, **48**, 2, 2273-2280.

12. Sara G. S. Santos, Larissa O. Paulista, Claudio Passalía, Belisa Alcantara Marinho, Marina Flores, Marisol D. Labas, Rodolfo J. Brandi, Vítor J. P. Vilar, "A step forward on NETmix reactor for heterogeneous photocatalysis: kinetic modeling of As(III) oxidation", *Chemical engineering journal*, 2021, **405**, 126612.

13. Ana Caroline Klemz *et al.* (14 authors), "Treatment of real oilfield produced water by liquid-liquid extraction and efficient phase separation in a mixer-settler based on phase inversion", *Chemical engineering journal*, 2021, **417**, 127926.

14. Klemen Bohinc, Erna Tintor, Davor Kovačević, Rajko Vidrih, Anamarija Zore, Anže Abram, Željka Kojić, Marija Obradović, Valentina Veselinović, Olivera Dolić, "Bacterial adhesion on glass-ionomer cements and micro/nano hybrid composite dental surfaces", *Coatings*, 2021, **11**, 2, 235.

15. Klemen Bohinc, Lora Kukić, Roman Štukelj, Anamarija Zore, Anže Abram, Tin Klačić, Davor Kovačević, "Bacterial adhesion capacity of uropathogenic *Escherichia coli* to polyelectrolyte multilayer coated urinary catheter surface", *Coatings*, 2021, **11**, 6, 630.

16. Tine Malgaj, Tadej Mirt, Andraž Kocjan, Peter Jevnikar, "The influence of nanostructured alumina coating on bonding and optical properties of translucent zirconia ceramics: in vitro evaluation", *Coatings*, 2021, **11**, 9, 1126.

17. Anže Abram, Anamarija Zore, Urban Lipovž, Anita Košak, Maja Garvas, Žan Boltežar, Klemen Bohinc, "Bacterial adhesion on prosthetic and orthotic material surfaces", *Coatings*, 2021, **11**, 12, 1469.

18. Calvin Cheung, Ilaria Monaco, Nina Kostevšek, Mauro Comes Franchini, Wafa Al-Jamal, "Nanoprecipitation preparation of low temperature-sensitive magnetoliposomes", *Colloids and surfaces. B, Biointerfaces*, 2021, **198**, 111453.

19. Ge Bian, Olga Ageeva, Aleksander Rečnik, Gerlinde Habler, Rainer Abart, "Formation pathways of oriented magnetite micro-inclusions in plagioclase from oceanic gabbro", *Contributions to Mineralogy and Petrology*, 2021, **176**, 12, 104.

20. Monika Kušter, Anton Meden, Boštjan Markoli, Zoran Samardžija, Maja Vončina, Pascal Boulet, Émilie Gaudry, Jean-Marie Dubois, Sašo Šturm, "Crystal structure, microstructure and electronic properties of a newly discovered ternary phase in the Al-Cr-Sc system", *Crystals*, 2021, **11**, 12, 1535.

21. Andraž Kocjan, Jasna Cotič, Tomaž Kosmač, Peter Jevnikar, "In vivo aging of zirconia dental ceramics - part I: biomedical grade 3Y-TZP", *Dental materials*, 2021, **37**, 3, 443-453.

22. Jasna Cotič, Andraž Kocjan, Sanja Panchevska, Tomaž Kosmač, Peter Jevnikar, "In vivo aging of zirconia dental ceramics - part II: highly-translucent and rapid-sintered 3Y-TZP", *Dental materials*, 2021, **37**, 3, 454-463.

23. Aline M. Novack *et al.* (12 authors), "Facile fabrication of hybrid titanium(IV) isopropoxide/pozzolan nanosheets (TnS-Pz) of high photocatalytic activity: characterization and application for Cr(VI) reduction in an aqueous solution", *Environmental science and pollution research international*, 2021, **28**, 23568-23581.

24. Iztok Naglič, Blaž Leskovar, Zoran Samardžija, Boštjan Markoli, "Influence of Ga on the formation of phases in cast Al-Mn-based alloys", *Intermetallics*, 2021, **136**, 107263.

25. Aybike Paksoy, Samira Fatma Kurtoğlu, Azam Khodadadi Dizaji, Zerrin Altintaş, Sina Khoshsima, Alper Uzun, Özge Balci, "Nanocrystalline cobalt-nickel-boron (metal boride) catalysts for efficient hydrogen production from the hydrolysis of sodium borohydride", *International journal of hydrogen energy*, 2021, **46**, 11, 7974-7988.

26. Matic Korent, Marko Soderžnik, Urška Ročnik, Sandra Drev, Kristina Žužek Rožman, Sašo Šturm, Spomenka Kobe, Kristina Žagar, "Toward low-energy spark-plasma sintering of Hot-deformed Nd-Fe-B magnets", *International journal of materials science and applications*, 2021, **10**, 5, 98-107.

27. Giulia Della Pelle, Andrea Delgado López, Marina Salord Fiol, Nina Kostevšek, "Cyanine dyes for photo-thermal therapy: a comparison of synthetic liposomes and natural erythrocyte-based carriers", *International journal of molecular sciences*, 2021, **22**, 13, 6914.

28. Maja Antanasova, Andraž Kocjan, Anže Abram, Janez Kovač, Peter Jevnikar, "Pre-oxidation of selective-laser-melted titanium dental alloy: effects on surface characteristics and porcelain bonding", *Journal of adhesion science and technology*, 2021, **35**, 19, 2094-2109.

29. Aljaž Iveković, Maria L. Montero-Sistiaga, Jef Vleugels, Jean-Pierre Kruth, Kim Vanmeensel, "Crack mitigation in laser powder bed fusion processed Hastelloy X using a combined numerical-experimental approach", *Journal of alloys and compounds*, 2021, **864**, 158803.

30. Kristina Žagar *et al.* (13 authors), "Microstructural insights into the coercivity enhancement of grain-boundary-diffusion-processed Tb-treated Nd-Fe-B sintered magnets beyond the core-shell formation mechanism", *Journal of alloys and compounds*, 2021, **864**, 158915.

31. Guanglong Ma *et al.* (20 authors), "PD1 blockade potentiates the therapeutic efficacy of photothermally-activated and MRI-guided low temperature-sensitive magnetoliposomes", *Journal of controlled release*, 2021, **332**, 419-433.

32. Kaja Križman, Saša Novak, Julijana Kristl, Gregor Majdič, Nataša Drnovšek, "Long-acting silk fibroin xerogel delivery systems for controlled release of estradiol", *Journal of drug delivery science and technology*, 2021, **65**, 102701.

33. Zerrin Altintaş, Sina Khoshsima, Marcus P. Schmidt, Matej Bobnar, Urlich Burkhardt, Mehmet Somer, Özge Balci, "Evolution of magnetic properties of crystalline cobalt-iron boride nanoparticles via optimization of synthesis conditions using hydrous metal chlorides", *Journal of Magnetism and Magnetic Materials*, 2021, **523**, 167634.

34. Tomaž Tomše, Jaćim Jaćimović, Jean-Marie Dubois, Spomenka Kobe, Kristina Žužek Rožman, Sašo Šturm, "Nanostructured multicomponent Nd-Fe-B magnets prepared by a spark-plasma-sintering approach", *Journal of Magnetism and Magnetic Materials*, 2021, **553**, 168011.

35. Milan Vukšić, Irena Žmak, Lidija Ćurković, Danko Ćorić, Petra Jenuš, Andraž Kocjan, "Evaluating recycling potential of waste alumina powder for ceramics production using response surface methodology", *Journal of Materials Research and Technology*, 2021, **11**, 866-874.

36. Guiomar D. Soria *et al.* (11 authors), "Uncorrelated magnetic domains in decoupled $SrFe_{12}O_{19}/Co$ hard/soft bilayers", *Journal of physics. D, Applied physics*, 2021, **54**, 5, 054003.

37. Petra Jenuš, Aleksander Učakar, Sandra Repše, Claudio Sangregorio, Michele Petrecca, Martin Albino, Riccardo Cabassi, César De Julián Fernández, Blaž Belec, "Magnetic performance of $SrFe_{12}O_{19} - Zn_{0.2}Fe_{2.8}O_4$ hybrid magnets prepared by Spark Plasma Sintering", *Journal of physics. D, Applied physics*, 2021, **54**, 20, 204002.

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39. Nina Kostevšek, Patricija Miklavc, Matic Kisovec, Marjetka Podobnik, Wafa Al-Jamal, Igor Serša, "Magneto-erythrocyte membrane vesicles' superior T_2 MRI contrast agents to magneto-liposomes", *Magnetochemistry*, 2021, **7**, 4, 51.

40. Roman Celin, Fevzi Kafexhiu, Grega Klančnik, Jaka Burja, "Properties of the simulated coarse-grained microstructure of quenched and tempered high-strength steel", *Materiali in tehnologije*, 2021, **55**, 1, 115-120.

41. Carlo Burkhardt, Antje Lehmann, Peter Fleissner, Laura Grau, Mirko Trautz, Maximilian Mungenast, Benjamin Podmiljšak, Spomenka Kobe, "Comparative evaluation of anti-corrosion coatings for NdFeB-type magnets with respect to performance and recyclability via hydrogen-assisted recycling (HPMS)", *Materials proceedings*, 2021, **5**, 1, 87.

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43. Igor Velkavrh, Joel Voyer, Fevzi Kafexhiu, Bojan Podgornik, "Creep rate, friction, and wear of two heat-affected zone regions of 9-12 wt.% Cr steels", *Metals*, 2021, **11**, 4, 558.

44. Barbara Kalebić, Jelena Pavlović, Jelena Dikić, Aleksander Rečnik, Sašo Gyergyek, Nikola Škoro, Nevenka Rajić, "Use of natural clinoptilolite in

the preparation of an efficient adsorbent for ciprofloxacin removal from aqueous media", *Minerals*, 2021, **11**, 5, 518.

45. Mirjam Gorjan, Petra Virant, Franc Rojko, Anže Abram, Rebeka Rudolf, Peter Raspor, Anamarija Zore, Klemen Bohinc, "Bacterial adhesion of *Streptococcus mutans* to dental material surfaces", *Molecules*, 2021, **26**, 4, 1152.

46. Mirko Maturi, Erica Locatelli, Letizia Sambri, Silvia Tortorella, Sašo Šturm, Nina Kostevšek, Mauro Comes Franchini, "Synthesis of ultrasmall single-crystal gold-silver alloy nanotriangles and their application in photothermal therapy", *Nanomaterials*, 2021, **11**, 4, 912.

47. Hermina Hudelja, Thomas Konegger, Bernd Wicklein, Janko Čretnik, Farid Akhtar, Andraž Kocjan, "Freeze-casting of highly porous cellulose-nanofiber-reinforced γAl_2O_3 monoliths", *Open ceramics*, 2021, **5**, 100069.

48. Milan Vukšić, Irena Žmak, Lidija Ćurković, Andraž Kocjan, "Spark plasma sintering of dense alumina ceramics from industrial waste scraps", *Open ceramics*, 2021, **5**, 100076.

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52. Letiane Thomas Hendges *et al.* (10 authors), "Adsorption and desorption of water-soluble naphthenic acid in simulated offshore oilfield produced water", *Process safety and environmental protection*, 2021, **145**, 262-272.

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54. Pierre Van Cauwenbergh, Vahid Samaee, Lore Thijs, Jitka Nejezchlebová, Petr Sedlak, Aljaž Iveković, Dominique Schryvers, Brecht Van Hooreweder, Kim Vanmeensel, "Unravelling the multi-scale structure-property relationship of laser powder bed fusion processed and heat-treated $AlSi_{10}Mg$", *Scientific reports*, 2021, **11**, 6423.

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59. Tjaša Matjašič, Tatjana Simčič, Tjaša Kanduč, Zoran Samardžija, Nataša Mori, "Presence of polyethylene terephthalate (PET) fibers in hyporheic zone alters colonization patterns and seasonal dynamics of biofilm metabolic functioning", *Water Research*, 2021, **203**, 117455.

REVIEW ARTICLE

1. Dimitrij Ješić, Damjan Lašič Jurković, Andrej Pohar, Luka Suhadolnik, Blaž Likozar, "Engineering photocatalytic and photoelectrocatalytic CO_2 reduction reactions: mechanisms, intrinsic kinetics, mass transfer resistances, reactors and multi-scale modelling simulation", *Chemical engineering journal*, 2021, **407**, 126799.

2. Giulia Della Pelle, Nina Kostevšek, "Nucleic acid delivery with red-blood-cell-based carriers", *International journal of molecular sciences*, 2021, **22**, 10, 5264.

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5. Cecilia Granados-Miralles, Petra Jenuš, "On the potential of hard ferrite ceramics for permanent magnet technology: a review on sintering strategies", *Journal of physics. D, Applied physics*, 2021, **54**, 3, 303001.

6. Ipeknaz Özden, Aljaž Iveković, Andraž Kocjan, "Additive manufacturing of ceramics from thermoplastic feedstocks", *Open ceramics*, 2021, **6**, 100129.

PUBLISHED CONFERENCE CONTRIBUTION

1. Patrick Seleš, Žiga Lipovšek, Martina Kocijan, Tina Radošević, Damjan Vengust, Matejka Podlogar, "Synthesis of ZnO powders with different morphologies for photocatalytic degradation", In: *56th International Conference on Microelectronics, Devices and Materials & the Workshop on Personal Sensors for Remote Health Care Monitoring, 22-24 September 2021, Ljubljana, Slovenia*, Proceedings, MIDEM, 2021, 35-42.

2. Anubhav Vishwakarma, Matej Komelj, "Design of a smart-phone self-charger, based on a permanent magnet", In: *56th International Conference on Microelectronics, Devices and Materials & the Workshop on Personal Sensors for Remote Health Care Monitoring, 22-24 September 2021, Ljubljana, Slovenia*, Proceedings, MIDEM, 2021, 52-56.

INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Nina Kostevšek, Igor Serša, "Characterization of metal-based nanoparticles as contrast agents for magnetic resonance imaging", In: *Analysis and characterisation of metal-based nanomaterials*, (Comprehensive analytical chemistry **93**), Elsevier, 2021, 303-343.

2. Andraž Kocjan, Tadej Mirt, Ralf-Joachim Kohal, Zhijian Shen, Peter Jevnikar, "Zirconia ceramics: clinical and biological aspects in dentistry", In: *Encyclopedia of materials: technical ceramics and glasses*, Elsevier, 2021, **3**, 817-832.

3. Slavko Bernik, "Oxide thermoelectric materials: compositional, structural, microstructural, and processing challenges to realize their potential", In: *Thermoelectric energy conversion: theories and mechanisms, materials, devices, and applications*, (Woodhead publishing series in electronic and optical materials), Woodhead Publishing, 2021, 269-302.

PATENT

1. Saša Novak, Nataša Drnovšek, Gregor Murn, *Implant having a multilayered coating and a process for preparing thereof*, EP2595669 (B1), European Patent Office, 13. 10. 2021.

2. Xuan Xu, Sašo Šturm, Kristina Žužek Rožman, *A method for recovery of $Nd_2Fe_{14}B$ grains from bulk sintered Nd-Fe-B magnets and/or magnet scraps by electrochemical etching*, EP3660174 (B1), European Patent Office, 27. 10. 2021.

3. Sašo Gyergyek, Andraž Kocjan, Darko Makovec, *Method for synthesis of coated magnetic particles*, GB2582272 (B), Intellectual Property Office, 14. 07. 2021.

4. Simon Reinhard, Jaćim Jaćimović, Lorenz Herrmann, Tomaž Tomše, *Method of producing a permanent magnet with inter-grain heavy-rare-earth element*, EP3649659 (B1), European Patent Office, 07. 04. 2021.

THESES AND MENTORING

1. Hermina Hudelja, *Freeze casting of hierarchically structured highly porous $\gamma - Al_2O_3$ monoliths:* doctoral dissertation, Ljubljana, 2021 (mentor Andraž Kocjan).

2. Matic Korent, *Processing of heavy-rare-earth-lean Nd-Fe-B permanent magnets for high-temptrature applications:* doctoral dissertation, Ljubljana, 2021 (mentor Kristina Žagar Soderžnik; co-mentor Spomenka Kobe).

3. Sara Tominc, *Charge compensation mechanisms and twinning in doped SnO_2-based ceramics:* doctoral dissertation, Ljubljana, 2021 (mentor Aleksander Rečnik; co-mentor Nina Daneu).

DEPARTMENT FOR MATERIALS SYNTHESIS   K-8

The research of the Department for Materials Synthesis is mainly related to the synthesis of advanced materials, especially magnetic materials. Special attention is given to nanostructured materials, such as ferrofluids, functionalized nanoparticles for use in biomedicine, multifunctional nanocomposites, catalysts, and fluorescent nanoparticles.

Head:
Prof. Darko Makovec

A large part of research at the Department for Materials Synthesis is devoted to the synthesis of nanoparticles. In 2021 we continued our research devoted to the hydrothermal synthesis and structural characterization of bismuth titanate ($Bi_4Ti_3O_{12}$, BIT) nanoparticles. Depending on the experimental conditions (e.g., the concentration of NaOH) BIT can be synthesized in the form of either nanoplatelets or nanowires. The structure of BIT nanoparticles was thoroughly characterized using atomic-resolution imaging with a C_S-probe-corrected scanning-transmission electron microscope (cooperation with Prof. Goran Dražić, National Institute of Chemistry) in combination with X-ray diffractometry (cooperation with Prof. Anton Meden, Faculty of Chemistry and Chemical Technology, University of Ljubljana) and Raman spectroscopy. We found that the nanoplatelets (10 nm thick and 50–200 nm wide) exhibit the Aurivillius-type layered-perovskite crystal structure that is characteristic of BIT, whereas the nanowires (15–35 nm wide and from several hundreds of nm to several μm long) exhibit an entirely new structure with an orthorhombic unit cell. A tentative structural model was proposed (Figure 1). The nanowire structure is composed of two structural layers alternating along the orthorhombic c-direction: a structural layer composed of two parallel layers of Bi atoms that resemble the $(Bi_2O_2)^{2+}$ layer of the Aurivillius structure, and a structural layer composed of two parallel layers of Ti atoms, where every sixth Ti is replaced with Bi. Observations of the ferroelectric domains with transmission electron and piezo-response force microscopy (cooperation with Hana Uršič, Department for Electronic Ceramics) indicated the ferroelectric nature of both nanostructures. In 2021 we focused on processes leading to the formation of two distinct morphologies of BIT nanoparticles. The hydrothermal treatment for 38 hours at 200 °C led to the formation of the nanowires with a metastable orthorhombic structure and the nanoplatelets with an equilibrium Aurivillius layered-perovskite structure at lower (1 mol/L) and higher (>1 mol/L) NaOH concentrations, respectively. At the initial stage of hydrothermal synthesis a mixture of two metastable polymorphs was formed: the nanowires and the highly defected perovskite phase. The perovskite phase in the form of globular aggregates of nanocrystallites only contained Bi^{3+} and Ti^{4+} cations (Na^+ or Ti^{3+} were not detected). In the continuation of the hydrothermal treatment, the aggregates of perovskite nanocrystals dissolved in the lower NaOH concentrations, whereas in the higher NaOH concentrations the nanowires dissolved, while the Aurivillius nanoplatelets grew from the surfaces of the perovskite aggregates (Figure 3).

Discovery of a new crystal structure, a metastable polymorph of $Bi_4Ti_3O_{12}$ stabilized at the nanoscale in the form of nanowires.

In 2021 we started a cooperation with researchers from Faculty of Electrical Engineering, University of Ljubljana (group of Prof. Damijan Miklavčič) in the framework of a national project devoted to selective electroporation by distributed nanoelectrodes. We developed methods for the synthesis of gold nanoparticles with controllable size and shape (Figure 3). The gold nanoparticles were then coated with a layer of silica with different morphologies. The coating process was based on our dynamic soft-templating method that allows the simple design of applicable silica shells containing tuneable pore geometries with pore sizes ranging from below 5 nm to above 40 nm. The method was published in ACS Applied Materials & Interfaces (IF= 9.229) in 2021. Moreover, a dynamic soft-templating strategy was developed to controllably synthesize hierarchical, dual-mesoporous silica shells on various magnetic nanoparticles, in terms of nanoparticle dimension (i.e., from 3 nm to a micrometre), shape (i.e., spherical, chain-like, and disc-like), and magnetic properties (i.e., permanently magnetic and superparamagnetic). This method can serve as a general approach to the fabrication of well-designed mesoporous silica coatings on a wide variety of core nanoparticles, as demonstrated using the gold nanoparticles.

Apart from the silica coating, the functionalization molecules can be grafted onto the nanoparticles' surfaces to control their surface properties. The layer of molecules has to be bonded by forming stable covalent bonds, not

Figure 1: Ferroelectric $Bi_4Ti_3O_{12}$ nanoparticles can be hydrothermally synthesized in two distinct morphologies, i.e., nanoplatelets and nanowires. The nanowires exhibit a new, layered crystal structure that has not been described before.

Development of new, magnetically guidable drug-delivery systems.
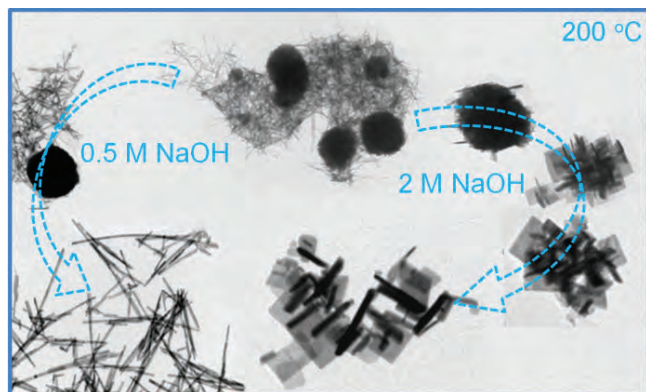
Figure 2: A mixture of two metastable polymorphs of bismuth titanate forms in the initial stages of the hydrothermal treatment of precipitated Bi³⁺ and Ti⁴⁺ ions in NaOH: nanowires with an orthorhombic structure and globular aggregates of perovskite crystallites. In the next stage, the perovskite aggregates dissolve at lower NaOH concentrations, whereas at the higher NaOH concentrations the nanowires dissolve, while the nanoplatelets with an equilibrium Aurivillius structure start to grow from the surfaces of the perovskite aggregates.

Synthesis of magneto-optic Janus nanoplatelets prepared from barium hexaferrite nanoplatelets and gold nanoparticles with Pickering emulsions.

Figure 3: TEM images of gold nanoparticles: spherical nanoparticles (left-side image) and gold nanorods (right-side image).

to be desorbed or exchanged with other ligands from the medium. Since irreversible covalent bonding is not possible between ionic inorganic surfaces and organics an alternative coordinative bonding is often exploited for the surface functionalisation. Very strong coordinative bonding can be achieved between surface metal ions and some organic moieties (e.g., carboxylates, catechols, phosphonates). Our results showed that by coating superparamagnetic maghemite nanoparticles with some catechols the saturation magnetization of the nanoparticles increased. This was opposite to the expected decrease because of the nonmagnetic coating. On the other hand, a much larger decrease in the saturation magnetization of barium hexaferrite nanoplatelets was measured than expected from the fraction of a tetraphosphonate coating. Among all the studied phosphonate ligands (mono-, di- and bisphosphonates) only the tetraphosphonate ligand showed such an effect. To elucidate such unexpected behaviour, a detailed spectroscopic study in collaboration with Prof. Iztok Arčon (University of Nova Gorica) and theoretical calculations by Dr Layla Martin Samos, Dr Matic Poberžnik and Gabriela Herrero (CNR, Trieste) have been considered.

We continued the research related to the ferromagnetic suspensions of barium hexaferrite nanoplatelets (in cooperation with the Department of Complex Matter). We focused on understanding the colloidal interactions in suspensions of the hexaferrite nanoplatelets in isotropic solvents using different surface ligands, including various phosphonates and nonpolar ligands for making nonpolar ferrofluids based on the nanoplatelets. We determined conditions for the formation of ferromagnetic ferrofluids in isotropic solvents and the stability range of ferromagnetic liquid crystals.

A new research direction evolved from our background on the hexaferrite nanoplatelets and ferrofluids. Our aim is to add to the magnetic and shape anisotropy of those special materials by introducing additional functionality only on one basal surface of the nanoplatelets, thus making Janus nanoplatelets. One of the studies is related to the development of magneto-photonic barium-hexaferrite - gold Janus nanoplatelets in the frame of a Seal of Excellence project "Multifunctional Janus Nanoplatelets" (led by Dr Jelena Papan). The first barium hexaferrite - gold Janus nanoplatelets were obtained via a Pickering emulsion system.

A national project with the Faculty of Chemistry and Chemical Technology, University of Ljubljana is focused on the development of the hybridization technology for making magneto-electric Janus nanoplatelets based on the immobilization of the barium-hexaferrite nanoplatelets on a solid substrate. The immobilized monolayer of nanoplatelets will allow for their hybridization with electrically polar ligands only on one basal surface of the nanoplatelets. A major focus in 2021 was on the optimization of glass-substrate functionalization. We identified vapour-phase deposition as the most efficient method for the amino-functionalized glass-substrates. In parallel, optical absorption and fluorescence methods were adopted to assess the density of active amine groups at glass surfaces.
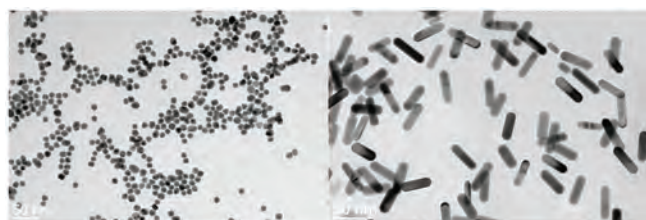
We were also very active within the FET-OPEN MAGNELIQ project where we cooperate with University of Maribor, CNR Trieste, Czech Academy of Sciences and a SME Prensilia from Pisa. In the project we aim to develop a magneto-electric liquid based on magneto-electric Janus nanoplatelets. We studied the coordinative interaction of complexing ligands with barium-hexaferrite nanoplatelets. Our aim was to identify conditions ensuring stable magneto-electric hybrids. Experimental studies run in parallel with theoretical calculations of basic interaction potentials. In addition, a variety of ferromagnetic liquids with a strong magneto-optic response was prepared and characterized.

We continued the research on the preparation of new drug-delivery systems based on clusters of superparamagnetic nanoparticle (i.e., nanoclusters). Their magnetic guidance enables a broad spectrum of applications, not only for magnetic drug delivery, but also for magnetic separation, magnetic particle imaging, magnetic resonance imaging, etc. In 2021 we demonstrated the platform for drug delivery based on magnetic nanoparticles. We have developed partially hollow magnetic nanostructures that have nanoscale voids available for drug loading, while they preserve sufficient magnetic responsiveness. This interdisciplinary collaborative work was performed with researchers from the Faculty of Pharmacy, University of Ljubljana (Prof. Petra Kocbek). As an alternative, we also

developed delivery particles with a space for drug loading available in the compartments of radially aligned pores within the silica shell on the magnetic particles. The nanoclusters were coated with silica with the large and radially aligned pores, which enable loading of an active pharmaceutical substance, while the particle core provides magnetic guidance of the loaded drug to a targeted tissue. The research on this topic is in progress.

In 2021 we also continued a close collaboration with researchers from the Department of Chemical and Pharmaceutical Sciences, University of Trieste, Italy (Prof. Silvia Marchesan). We successfully demonstrated the formation of hybrid nanomaterials made of self-assembled di- and tripeptides. The composite material forms different nanostructures with diverse properties. Our future efforts will focus upon the extension of this chemical platform to biocompatible materials able to perform time-controlled drug release. Furthermore, our intense collaboration with this group was continued on the development of magnetic nanostructures conjugated with short peptides and self-assembled fibrillar peptide nanostructures. Controlling the magneto-mechanical effect of anisotropic magnetic particles on soft and fragile peptide fibrils was our central research interest.

We continued our research on the application of the magnetic heating of carbon- or alumina-coated magnetic nanoparticle clusters in catalysis. For the synthesis of the nanostructured carbon-coated nanoclusters the magnetic nanoparticles were coated with a precursor using the hydrothermal carbonization of carbohydrates followed by thermal treatment. The synthesis procedure for the nanostructured alumina-coated clusters was developed in cooperation with the Department for Nanostructured Materials based on the deposition of a precursor material with the hydrolysis of AlN in a colloidal suspension of superparamagnetic iron-oxide nanoparticles, followed by a thermal treatment.

In cooperation with the Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry (Dr Blaž Likozar and Dr Miha Grilc) we studied the AC-field-mediated catalysis using Ru-bearing carbon-coated magnetic nanoclusters. The catalyst exhibited a large surface area and was homogenously decorated with small Ru nanoparticles, approximately 2 nm in size. The catalyst was used in the hydrotreatment of levulinic acid. The yield of γ-valerolactone reached 100 % under mild conditions (total pressure of 1 MPa maintained with H_2) within 1 hour of magnetic heating. The in-depth analysis and modelling of the hydrogenation and deoxygenation processes showed that the surface of the catalyst rapidly heats to 137 °C, while the bulk of the medium remains at the significantly lower temperature of 85 °C. Such a thermal imbalance increased the rate of conversion of the isopropyl levulinate (formed by the competing reaction) to γ-valerolactone and thus increasing the yield. Such an analysis rationalizes experimental observations and provides a solid background for further optimization of the process. In addition, the catalyst showed remarkable stability, since after four recyclings the conversion and selectivity remained practically unchanged.

Figure 4: BF STEM image of magnetic Co_xNi_{1-x} nanoparticles embedded within a nanostructured alumina matrix.

In collaboration with the same group from National Institute of Chemistry we studied the influence of the size and size distribution of catalytic Ru nanoparticles on their activity for the hydrogenation of hydroxymethyl furfural (HMF) and in the decomposition of NH_3. A series of Ru-bearing carbon-coated magnetic nanoclusters was prepared while the size of the Ru nanoparticles was varied from 0.9 to approx. 5 nm. The in-depth analysis and modelling of the hydrogenation of HMF showed that the smallest Ru nanoparticles exhibit the highest activity and selectivity for 2,5-bishydroxymethalfuran (BHMF). Their small size most likely facilitates the preferential adsorption of the HMF molecule through the aldehyde group. In such a configuration the ring saturation is inhibited, thereby improving selectivity. In stark contrast, the same catalyst was only poorly active in the decomposition of NH_3. Here, the highest activity was observed when the Ru nanoparticles were approximately 2 nm in diameter. Our best catalyst demonstrated remarkable activity in temperature-ramping experiments. The decomposition onset temperature was found to be 330 °C, while the full conversion of NH_3 was achieved at only marginally higher temperatures. Such a low temperature shows high potential for the applications of the developed catalysts in on-demand H_2 production through the decomposition of NH_3.

Actuation of magnetic nanoclusters with an AC magnetic field was applied to selectively heat the surface of a catalyst.

We have also been very active in the H2020 project Oracle, which aims to develop the scalable and flexible electrified production of NH_3 for fuel applications. Here we collaborate with several European institutions focusing on catalysts' development and their integration within reactor units utilizing the magnetic heating of coated magnetic nanoclusters for flexible and on-demand production. We have developed a scalable aqueous method for the preparation of Co_xNi_{1-x} precursor particles based on co-precipitation and subsequent hydrothermal treatment

to improve the homogeneity of their composition. Such nanoparticles were successfully embedded within the alumina matrix using our method based on the hydrolysis of AlN (Figure 4). During high-temperature reduction the precursor nanoparticles reduce to Co_xNi_{1-x} nanoparticles. The developed method enables control of the composition and thus control over the magnetic properties of the nanoparticles. They showed only a marginal decrease in the magnetization as a consequence of surface oxidation after prolonged time under an air atmosphere. Under reducing conditions, the properties are fully restored. What is more important is that they show good heating under an AC-field even under technologically relevant conditions, i.e., in a H_2 flow.

We also continued with the research of fluorescent optical materials. Fluorescent nanoparticles with up-conversion emission can be applied in various optical elements and are also proposed as alternative bio-markers in imaging diagnostic techniques for medicine. After our previous discovery of the significant dissolution of fluoride-based up-converting nanoparticles (UCNPs; e.g., Ln-doped LnF_3 and $NaYF_4$) we focused on the prevention/minimization of their dissolution. We studied the efficiency of some phosphonate coatings to prevent the dissolution of the UCNPs. We showed that the phosphonate structure and coating-synthesis conditions are very important in the definition of the density of phosphonic coatings. The dissolution studies were made in cooperation with the Department of Inorganic Chemistry and Technology (Dr Maja Ponikvar-Svet) and the Czech Academy of Sciences (Dr Uliana Kostiv). All the studies were supported with optical characterization in cooperation with the Department of Complex Matter (Prof. Boris Majaron) and with cell-viability studies at the Faculty of Medicine, University of Ljubljana (Dr Lovro Žiberna). Some of the results formed part of the MSc thesis of Maša Vozlič, who received Prešern's award from the University of Ljubljana and Krka's award from Krka company.

We also continued our research of materials displaying a positive temperature coefficient of resistivity (PTCR). The focus was on composite materials containing a mixture of a conducting phase (metal) and a non-conducting phase ($BaTiO_3$ ceramics). Due to dimensional changes during a phase transformation in the non-conducting phase, disconnections occur in the conductive phase that led to the PTCR anomaly.

Some outstanding publications in the past year

1. Nemec, Sebastjan, Kralj, Slavko. A versatile interfacial coassembly method for fabrication of tunable silica shells with radially aligned dual mesopores on diverse magnetic core nanoparticles. ACS applied materials & interfaces, ISSN 1944-8244, 2021, vol. 13, iss. 1, str. 1883-1894, ilustr., doi: 10.1021/acsami.0c17863.
2. Papan, Jelena, Hribar, Patricija, Mertelj, Alenka, Lisjak, Darja. Preparation of barium-hexaferrite/gold Janus nanoplatelets using the pickering emulsion method. Nanomaterials, ISSN 2079-4991. [Online ed.], 2021, vol. 11, no. 11, str. 2797-1-2797-18, doi: 10.3390/nano11112797.
3. Masdeu, Gerard, Findrik, Zvjezdana, Kralj, Slavko, Makovec, Darko, López-Santín, Josep, Álvaro Gregorio, G. Multi-reaction kinetic modeling for the peroxidase-aldolase cascade synthesis of a D-fagomine precursor. Chemical Engineering Science, ISSN 0009-2509. [Print ed.], 2021, vol. 239, str. 116602-1-116602-11.

Awards and Appointments

1. Sebastjan Nemec was awarded 2nd place in the Best student presentation competition at the SCS Annual Meeting 2021 conference in Portorož (22. – 24.9.2021)

Organization of conferences, congresses and meetings

1. Project Consortium Meeting H2020-FETOPEN-2018-2019-2020: MAGNELIQ, Ljubljana, 14. –15.10.2021

Patent granted

1. Sašo Gyergyek, Andraž Kocjan, Darko Makovec, Method for synthesis of coated magnetic particles, GB2582272 (B), Intellectual Property Office, 14. 07. 2021.

INTERNATIONAL PROJECTS

1. COST CA18132; Functional Glyconanamaterials for the Development of Diagnostics and Targeted Therapeutic Probes
Asst. Prof. Slavko Kralj
Cost Association Aisbl
2. H2020 - BeMAGIC; Magnetoelectrics Beyond 2020: A Training Programme on Energy-Efficient Magnetoelectric Nanomaterials for Advanced Information and Healthcare Technologies
Prof. Darja Lisjak
European Commission

3. H2020 - ORACLE; Novel Routes and Catalysts for Synthesis of Ammonia as Alternative Renewable Fuel
Asst. Prof. Sašo Gyergyek
European Commission
4. H2020 - PASSENGER; Pilot Action for Securing a Sustainable European Next Generation of Efficient RE-Free Magnets
Prof. Darko Makovec
European Commission
5. H2020 - MAGNELIQ; A Magneto-Electric Liquid - Better Sensing

Prof. Darja Lisjak
European Commission

RESEARCH PROGRAMME

1. Advanced inorganic magnetic and semiconducting materials
   Prof. Darko Makovec

R&D GRANTS AND CONTRACTS

1. Bactericidal nanoblades: a proof-of-concept approach for bimodal chemo-mechanicaleradication of persistent biofilms
   Asst. Prof. Slavko Kralj

2. Selective electroporation by distributed nanoelectrodes
   Asst. Prof. Slavko Kralj
3. Multifunctional Janus Nanoplatelets
   Jelena Papan
4. Liquid Magnets: fundamental studies of ferromagnetic order in liquids
   Prof. Darja Lisjak
5. Surface-selective hybridization technology for magneto-electric hybrids
   Prof. Darja Lisjak
6. Magneto Responsive Surfaces for Manipulation of Light and Liquids
   Prof. Darko Makovec
7. Magnetically-controllable nanocarriers mimicking endogenous lipid particles for improved drug/nanoparticle delivery
   Prof. Darko Makovec
8. Exploitation of the magneto-mechanical effect in the treatment of neurodegenerative diseases
   Asst. Prof. Slavko Kralj

VISITORS FROM ABROAD

1. Dr Vladimira Novotna, Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic, 14.-15. 10. 2021
2. Tomas Landovsky, Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic, 14.-15. 10. 2021
3. Dr Layla Martin Samos, Consiglio Nazionale delle Ricerche, Istituto Officina dei Materiali, Trieste, Italy, 14.-15. 10. 2021
4. Dr Nicolas Salles, Consiglio Nazionale delle Ricerche, Istituto Officina dei Materiali, Trieste, Italy, 14.-15. 10. 2021
5. Dr Matic Pobrežnik, Consiglio Nazionale delle Ricerche, Istituto Officina dei Materiali, Trieste, Italy, 14.-15. 10. 2021
6. Dr Gabriela Herrero, Consiglio Nazionale delle Ricerche, Istituto Officina dei Materiali, Trieste, Italy, 14.-15. 10. 2021
7. Miha Gunde, Consiglio Nazionale delle Ricerche, Istituto Officina dei Materiali, Trieste, Italy, 14.-15. 10. 2021
8. Francesco Clemente, Prensilia S.r.l, Pontedera, Italy, 14.-15. 10. 2021
9. Giulia Lippi, Prensilia S.r.l, Pontedera, Italy, 14.-15. 10. 2021
10. Nicola Motzo, Prensilia S.r.l, Pontedera, Italy, 14.-15. 10. 2021
11. Amadeo Morandi, Prensilia S.r.l, Pontedera, Italy, 14.-15. 10. 2021

STAFF

Researchers
1. Asst. Prof. Sašo Gyergyek
2. Asst. Prof. Slavko Kralj
3. Prof. Darja Lisjak
4. **Prof. Darko Makovec, Head**
5. Dr. Igor Zajc

Postdoctoral associates
6. Dr. Stanislav Čampelj
7. Dr. Jelena Papan
8. Dr. Ali Tufani

Postgraduates
9. Nina Križaj, B. Sc.
10. Sebastjan Nemec, B. Sc.
11. Žiga Ponikvar, B. Sc.
12. Anja Sedminek, B. Sc.
13. Luka Skubic, B. Sc.

Technical officer
14. Tina Černič, B. Sc.

Technical and administrative staff
15. Bernarda Anželak, B. Sc.
16. Tamara Matevc, B. Sc.

BIBLIOGRAPHY

ORIGINAL ARTICLE

1. Sebastjan Nemec, Slavko Kralj, "A versatile interfacial coassembly method for fabrication of tunable silica shells with radially aligned dual mesopores on diverse magnetic core nanoparticles", *ACS applied materials & interfaces*, 2021, **13**, 1, 1883-1894.
2. Ana Maria Garcia *et al.* (11 authors), "Nanoscale assembly of functional peptides with divergent programming elements", *ACS nano*, 2021, **15**, 2, 3015-3025.
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REVIEW ARTICLE

1. Črt Dragar, Slavko Kralj, Petra Kocbek, "Bioevaluation methods for iron-oxide-based magnetic nanoparticles", *International journal of pharmaceutics*, 2021, **597**, 120348.
2. C. De Julián Fernández, Claudio Sangregorio, Juan De la Figuera, Blaž Belec, Darko Makovec, Adrian Quesada, "Progress and prospects of hard hexaferrites for permanent magnet applications: topical review", *Journal of physics. D, Applied physics*, 2021, **54**, 15, 153001.
3. Slavko Kralj, Silvia Marchesan, "Bioinspired magnetic nanochains for medicine", *Pharmaceutics*, 2021, **13**, 8, 1262.

PUBLISHED CONFERENCE CONTRIBUTION

1. Anja Sedminek, Blaž Likozar, Sašo Gyergyek, "Novel routes and catalysts for synthesis of ammonia as alternative renewable fuel", In: *2. Interregional Congress H_2GreenTECH, 25 November 2021*, Follow up journal, Interreg Slovenija-Austria, 2021, 10-17.

PATENT

1. Sašo Gyergyek, Andraž Kocjan, Darko Makovec, *Method for synthesis of coated magnetic particles*, GB2582272 (B), Intellectual Property Office, 14. 07. 2021.

DEPARTMENT FOR ADVANCED MATERIALS K-9

At the Advanced Materials Department we investigate novel materials through an understanding of the mutual dependence of their structural, microstructural and functional characteristics. Modern technologies that enable the synthesis of materials with atomic and microscale precision are used to prepare pre-designed structural 3D materials, thin films and nanoparticles with the desired crystal structure, chemical composition, microstructure and morphology. Among our important objectives is the development of i) novel functional oxides for electronic applications and energy conversion, ii) antibacterial and piezoelectrical biocompatible materials and iii) heat-insulation materials with improved properties and sustainability.

Head:
Prof. Matjaž Spreitzer

Novel functional oxides

Two-dimensional (2D) materials are very important in the field of catalysis, as they present large surface areas with an ample number of active sites to boost the catalytic processes. However, the systematic design of 2D materials with the desired epitaxial properties remains a major scientific challenge. In this regard, understanding the nucleation and crystal-growth mechanisms becomes increasingly important and there is still a great lack of knowledge in this field. **2D materials** also present a unique opportunity to create **heterostructures with maximum face contact**, which can play crucial roles in reactions such as **photocatalytic hydrogen evolution**. In heterostructure photocatalysts with a well-ordered epitaxial interface, the interfacial electric field can contribute to the efficient separation of the photo-generated charge carriers and the preservation of a high redox ability. We addressed some of the challenges related to 2D photocatalysts by designing **$SrTiO_3$/$Bi_4Ti_3O_{12}$** heterostructure platelets through the hydrothermal topochemical conversion of $Bi_4Ti_3O_{12}$ template particles. These platelets were reported for enhanced hydrogen-evolution rates under simulated solar irradiation. Building up on this work, we have now obtained **new insights into the growth mechanism** of these heterostructure platelets, which will be used to propose the general design principles for the fabrication of similar 2D heterostructures. To be specific, we investigate how the reaction mechanism and morphology evolution can be controlled by balancing the lattice mismatch and supersaturation (Sr^{2+} and NaOH concentrations). Depending on the supersaturation, the conversion of $Bi_4Ti_3O_{12}$ platelets to $SrTiO_3$, under hydrothermal conditions, can yield three different morphologies: platelets, frames and cubes. We observed that **the quality of** the template **platelets** (such as particle dispersion, size distribution, etc.) greatly **influences the morphology** evolution and thus the growth mechanism. $Bi_4Ti_3O_{12}$ has a layered structure with alternatingly stacked pseudo-perovskite $[Bi_2Ti_3O_{10}]^{2-}$ blocks and bismuth-oxide $[Bi_2O_2]^{2+}$ layers. By means of STEM-HAADF we determined that the growth of $SrTiO_3$ perovskite occurs on the pseudo-perovskite part of the $Bi_4Ti_3O_{12}$ templates, while originally the $Bi_4Ti_3O_{12}$ templates are $[Bi_2O_2]^{2+}$ terminated. This implies that during the dissolution of $Bi_4Ti_3O_{12}$ in highly alkaline NaOH solution and heating to 200 °C, the $[Bi_2O_2]^{2+}$ layer dissolves, so the pseudo-perovskite layer is exposed as a substrate for the following growth. The optimized heterostructures were evaluated for noble-metal-free hydrogen evolution. Moreover, **new approaches were developed to achieve a higher surface area of as-prepared photocatalytic particles**, consequently **leading to an improvement** in the **hydrogen-evolution rate** by a factor of **100**.

In collaboration with the Chemical Engineering Department from the National Taiwan University, the studies of iso-propanol conversion over the $SrTiO_3$ and $SrTiO_3$/$Bi_4Ti_3O_{12}$ heterostructural platelets were performed to gain more understanding of the active-sites distribution and assess the application potential of these new platelets in heterogeneous catalysis. Depending of the acid-base properties of the catalysts' surface, the conversion of iso-propanol can proceed as dehydration on acid sites (formation of propene and water) or dehydrogenation on acid-base pairs (formation of acetone and hydrogen). Temperature programmed surface reactions revealed that **$SrTiO_3$-based platelets** are **more active** and **selective for the dehydrogenation reaction** compared to $SrTiO_3$ cubes and $SrTiO_3$ commercial powder, which non-selectively catalyze both reactions.

Other than these platelets, we have also developed **2D graphitic carbon nitride** (g-C_3N_4) **nanosheets for photocatalytic water-splitting**. Being a narrow-bandgap semiconductor (2.7 eV), g-C_3N_4 is one of the most promising low-cost photocatalysts discovered in the last decade. These nanosheets were developed and decorated with metal boride nanoparticles to improve their redox capability for the hydrogen-evolution reaction. In our preliminary results, at least **20-times-higher catalytic rates** are obtained for this novel composite. Likewise, we have also achieved
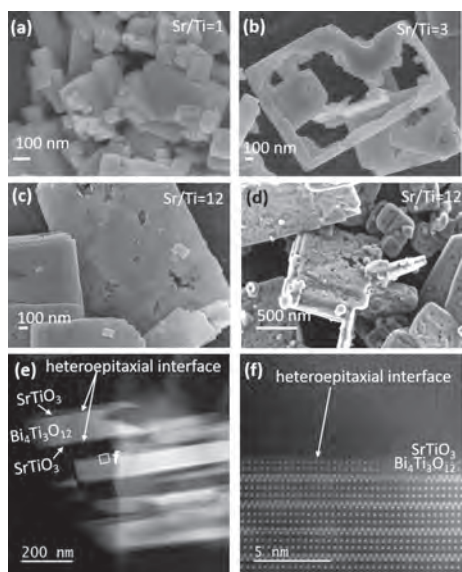
Figure 1: SEM micrographs of SrTiO$_3$ particles obtained from Bi$_4$Ti$_3$O$_{12}$ platelets after hydrothermal reaction in 6 mol/L NaOH at 200 °C for 12 hours with various initial Sr/Ti molar ratios (a: Sr/Ti=1, b: Sr/Ti=3, c and d: Sr/Ti=12) and with different starting temperatures of NaOH solution (a-c: 25 °C and d: 50 °C). (e) Low-magnification of HAADF-STEM image of edge-on-oriented SrTiO$_3$/Bi$_4$Ti$_3$O$_{12}$ heterostructural platelets at low stage of topochemical conversion (f) Atomic resolution Z-contrast image of SrTiO$_3$/Bi$_4$Ti$_3$O$_{12}$ heteroepitaxial contact, marked in Figure (e).
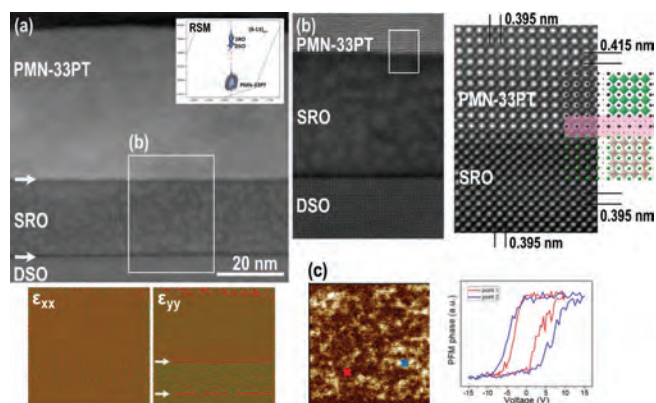
Figure 2: (a) Fully strained DSO/SRO/PMN-33PT heterostructure as confirmed by RSM analysis (upper right corner) and geometric phase analysis (GPA) of STEM image in the in-plane (ε_{xx}) and out-of-plane (ε_{yy}) directions. (b) Atomic-scale analysis of the SRO/PMN-33PT interface showing continuous perovskite lattice. (c) PFM out-of-plane amplitude and local PFM phase hysteresis loops measured in the two points marked on the image.

success in developing 2D structures of MoB$_2$, which is another promising multifunctional catalyst with applications in hydrogen generation (water electrolysis) and energy storage (batteries and supercapacitors).

A novelty in the field of integration of functional oxides with the help of pulsed laser deposition (PLD) technique is related to the **preparation of robust materials for the hydrogen (H$_2$) evolution in the photoelectrochemical water splitting system**. We achieved the simultaneous realization of the protection of the semiconductor substrate and the ease of charge transfers under the solar light illumination in the solution environment. The results showed that the **photogenerated current densities were greatly improved** compared to that measured under the dark condition, indicating the rapid photo response of our samples resulting from facile charge transportations between each junction. From an application point of view, such materials can be used for the fabrication of perovskite-reduced graphene oxide-silicon heterojunction devices.

Several research projects at our department are dedicated to tailoring the properties of thin films based on functional oxides. **Controlling the growth of complex relaxor ferroelectric thin films and understanding the relationship between biaxial strain–structural domain characteristics** are desirable for designing materials with a large electromechanical response. In this research field, we continued our studies of the effect of strain on the domain structure and functional response of thin films based on the relaxor ferroelectric (1-x) Pb(Mg$_{1/3}$Nb$_{2/3}$)O$_3$ – xPbTiO$_3$ (PMN–PT) solid solution. After optimization of the growth parameters and target compositions we succeeded to grow fully strained 40–45-nm thin epitaxial 0.67Pb(Mg$_{1/3}$Nb$_{2/3}$)O$_3$–0.33PbTiO$_3$ and 20-nm SrRuO$_3$ (PMN–33PT/SRO) heterostructures on singly terminated SrTiO$_3$ (ST) and ReScO$_3$ substrates (RSO) with Re=Dy, Tb, Gd, Sm, and Nd. All films were single phase with smooth 2D surfaces, as confirmed by *in situ* reflection high-energy electron diffraction (RHEED) and high-resolution X-ray diffraction (HR-XRD). Reciprocal space mapping (RSM) has revealed coherently strained films on all substrates, except on ST and NSO, where the films were partially relaxed. An example of a fully strained PMN–33PT/SRO heterostructure on a DyScO$_3$ (DSO) substrate with the largest compressive strain (-1.9%) induced in the films is shown in Figure 2. The analysis by high-resolution scanning transmission electron microscopy (HR-STEM) confirmed **homogeneous strain distribution in the film and atomically sharp interfaces without the presence of planar defects proving an epitaxial cube-on-cube growth mode of the PMN–33PT/SRO heterostructure**. The combined XRD RSMs and piezoresponse force microscopy (PFM) analysis revealed that the domain structure of the PMN–33PT heterostructures is sensitive to the applied compressive strain. Stabilization of relaxor domains is characteristic for mildly strained PMN–33PT layers, whereas a highly distorted tetragonal structure is present in films under high compressive strains. The results of this research work show that **epitaxial strain engineering can serve as an effective approach for tailoring and enhancing the functional properties in relaxor ferroelectrics**. More details can be found in the scientific paper by J. Belhadi *et al*. published in RSC Advances (doi: 10.1039/d0ra10107a).

In June 2021 we acquired an additional system for pulsed laser deposition (PLD). Two PLD systems are now available at our department and enable the preparation of thin films of different materials. The main components of the first PLD system are a simple vacuum system, a sample stage with a resistive heater that allows heating to 900 °C, and a target carrier with an option for scanning the targets during pulsed-laser ablation. In addition to the basic components already listed, the second PLD system is also equipped with an ion-getter pump, titanium sublimation pump and valves that help to achieve an **ultra-high-vacuum environment** (5 × 10^{-10} mbar), which is a special feature, compared to usual PLD systems. Apart from the resistive heater, a system for IR laser heating is also available, enabling substrate heating up to 1200 °C. The UHV PLD system is vacuum-connected to a glove box that allows the storage of reactive targets, a storage chamber for storing up to 12 samples, and an analytical system for temperature-programmed desorption (TPD). This PLD system can also be connected to a vacuum suitcase, which enables the transfer of samples to devices for structural and chemical analysis (XPS, JT-STM) located within other departments of the Institute. Both PLD systems are equipped with high-energy electron diffraction (RHEED) systems, which enable monitoring of thin layer growth and the structural analysis of the surfaces of prepared samples. We can use the existing KrF pulsed laser for the ablation of targets on both PLD systems by using additional optical elements for guiding the laser light.

The **main advantage** of using two separate PLD systems is the **possibility to simultaneously work on projects**, where **targets containing volatile materials**, such as lead for the growth of various piezoelectric thin films, are used, as well as on projects where maintaining an **ultra-high vacuum is crucial** as in the case of the integration of oxide films with semiconductor materials.

Figure 3: Left: UHV PLD, right: HV PLD system, in the back: UV laser with the optical cabinet.

Our research was also extended to the field of **a new type of lithium-ion batteries** with a **solid electrolyte** that are **safer**, **more stable**, and have **better energy density** and **capacity** in comparison to batteries with a liquid electrolyte. In the scope of our study, we prepared a ceramic electrolyte based on a double perovskite $Li_{3x}La_{2/3-x}TiO_3$ with A-site deficiency that is characterized by high ionic conductivity (10^{-3} Scm^{-1}). In samples prepared by the conventional solid-state sintering method, we determined the influence of synthesis conditions, La/Li ratio, and doping on the microstructure and functional properties. The results will help to understand **the mechanism of ionic conductivity** in $Li_{3x}La_{2/3-x}TiO_3$, which is very important for the application of this material in batteries.

Our research in the field of materials for electronic devices also includes **"upside-down" ceramic composites** based on a high ratio of strontium titanate filler ($SrTiO_3$, ST), coupled with the corresponding binder, lithium molybdate (Li_2MoO_4, LMO). Composites are prepared by the room-temperature fabrication (RTF) as a sustainable alternative to time- and energy-consuming high-temperature sintering of ceramics. Various physical parameters, wettability and contact between LMO and ST, as well as mechanical properties have been studied, depending on the different content of LMO binder. The obtained experimental results in the radio-frequency range (1MHz) showed a relative permittivity (ε_r) between 65 and 120 with dielectric losses (tan δ) from 0.002 to 0.05. Using the RTF method, between **20 and 40% of the dielectric constant of conventionally sintered ST ceramics was achieved**. Furthermore, the compatibility of ST functional ceramic with an organotitanate precursor, which acts as a binder was also studied. After the impregnation process, the **dielectric** and **mechanical properties** were further **improved**. The relative permittivity (ε_r) values of the untreated and impregnated ST/TiOx composites ranged from 80 to 120 with dielectric losses (tan δ) of 0.0035 to 0.0151. The particular properties can attract considerable attention for the utilization of LMO-ST composites in the industry of electroceramics.

Zinc is an essential micronutrient to human health, so massive food additives and medicines based on zinc gluconate are produced every year. Unfortunately, once expired, waste zinc gluconates are generally disposed with other garbage, causing an excessive influx of zinc ions into the environment which could deactivate the soil, affect the plant growth and cause the great damage to humans and animals. In order **to reduce environmental pollution** and the waste of zinc resources, we investigated **recycling of expired waste zinc gluconate as source for preparation of ZnO structures**. We used hydrothermal synthesis for their preparation and studied the influence of the synthesis parameters on their morphology. We found that depending on the temperature and time, different ZnO structures are obtained, ranging from hollow spheres to lace-like plates (Figure 4). All the obtained ZnO structures were micrometer sized, but composed of nanoparticles. The photocatalytic activities of ZnO structures were followed by the degradation of the methylene blue dye under the influence of UV light in aqueous solution. **Lace ZnO plates** showed **better photocatalytic activity** than hollow ZnO spheres.
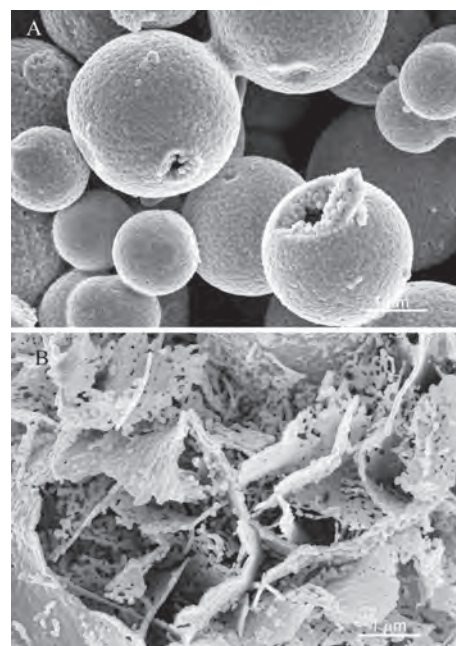
Figure 4: SEM image of ZnO (A) hollow spheres and (B) lace-like plates after firing.

Antibacterial and piezoelectric biocompatible materials

In collaboration with the Slovak Academy of Sciences we studied the **antibacterial activity of silver nanoparticles (AgNPs), synthesized via an environmentally friendly route**, i.e., by the reduction of silver nitrate ($AgNO_3$) in aqueous solutions that contained extracts of five different medicinal plants: *Berberis vulgaris*, *Brassica nigra*, *Capsella bursa-pastoris*, *Lavandula angustifolia* and *Origanum vulgare*. The synthesis procedure is rapid and simple and can be easily monitored via color changes and ultraviolet and visible (UV-Vis) spectroscopy. X-ray diffraction analysis (XRD) and transmission electron analysis (TEM) were used to confirm the formation of elemental silver nanoparticles (Figure 5). We showed that **the composition of the organic matrix** in terms of the anti-oxidant and total phenolic content **influences the size and morphology of the produced AgNPs**. Antimicrobial activity of the AgNPs was tested against five bacterial strains and it confirmed that **all the synthesized**
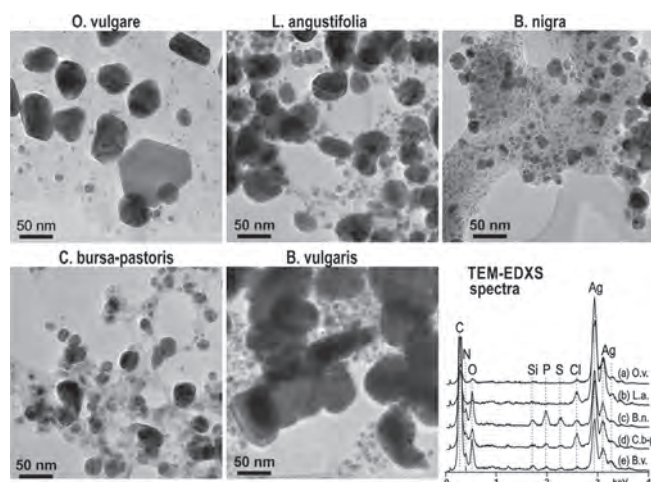
Figure 5: TEM images of the silver nanoparticles synthesized with different plant extracts from 5-mM AgNO$_3$. TEM/EDXS spectra taken across the AgNPs and the surrounding capping agents.
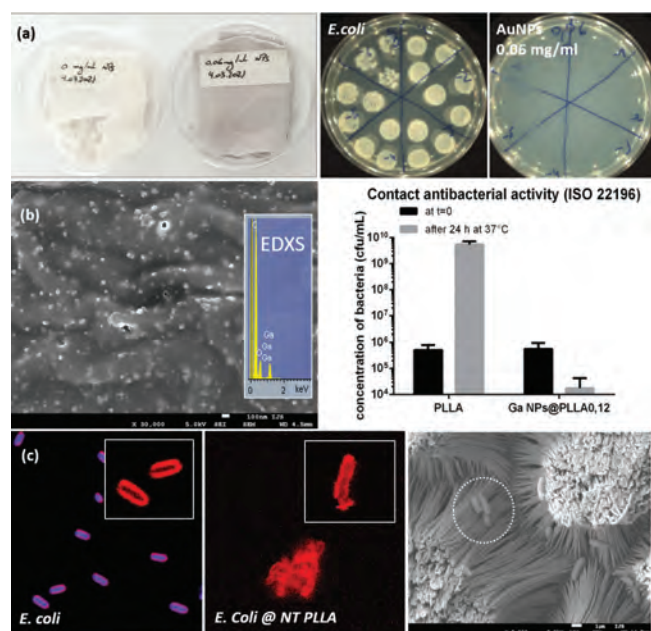
Figure 6: (a) Cotton functionalized with gold/arginine nanoparticles (AuNPs) and its bactericidal activity against E. coli; (b) poly-l-lactide (PLLA) films with gallium nanoparticles and their contact antimicrobial activity against P. aeruginosa; (c) damaging of membranes of bacteria (E. coli) after piezostimulation with nanotextured PLLA films.

nanoparticles exhibit enhanced antimicrobial activity in comparison to control, the best properties were observed for AgNPs prepared with *B. nigra* and *L. angustifolia* extracts. A paper by Salyova et al. was published in April 2021 in Nanomaterials (doi: 10.3390/nano11041005).

In the area of materials for biomedical applications, our work is focused on designing innovative tools for healing and tissue regeneration. For this purpose we are developing organic piezoelectric biomaterials and novel, more efficient antimicrobials. Within the project "Environmentally friendly antimicrobial material for textiles with improved properties", together with Centre for Technology Transfer (CTT) and in collaboration with Hungarian company Innowear-tex and Portugal industrial textile research institute (CITEVE), we developed a novel textile material formed of cotton and functionalized with gold/arginine nanoparticles (Au(arg)NPs). The testing confirmed the high stability of the AuNP-functionalized textile, which exhibited antibacterial activity (with a 6log10 reduction in *E. coli*) and antiviral activity (with 3log10 reduction in bacteriophages), even after 20 washing and drying cycles (Figure 6a). We used a similar approach for the functionalization of poly-l-lactide (PLLA) films with antimicrobial gallium. We have prepared composites of gallium nanoparticles with PLLA, which showed strong contact antibacterial activity against *P. aeruginosa* (with 6log10 reduction) (Figure 6b). When PLLA is processed as a piezoelectric film, it enables the non-specific targeting of bacterial cells with physical stimuli, which might be of great importance, particularly in the context of avoiding resistant bacterial strains. We have determined that such piezo-PLLA films, when fabricated as self-standing nanotubes, possess a high hydrogen peroxide degradation capacity. Moreover, they can damage bacterial membrane (Figure 6c). This effect was selective for bacterial membrane and no such damage was observed in human red blood cells, which is promising for the therapeutic use of such films. In this context, the synergy between the antimicrobial activity of the Ga nanoparticles and the piezoelectric matrix will be further explored to provide more effective antimicrobial activity against a wider range of bacterial strains.

Materials for heat-insulation applications

Improving the energy efficiency and sustainability are the core ideas of the circular economy and using obsolete materials to obtain products with added value presents a promising strategy. One such waste material is glass waste, which can be used for the production of foamed glass, a high-added-value product. A major disadvantage of the production of foamed glass is the high cost related to the step of adjusting the chemical composition of waste glass, which is necessary to obtain a product with superior properties. Additionally, the foaming mechanism is heavily influenced by the crystallization process, detrimentally affecting the quality of the final product.

In our research we studied the possibility to control undesired crystallization during the foaming of waste glass. We report on foamed glass production based on container glass cullet, foaming couple (carbon/Mn$_3$O$_4$) and crystallization inhibitors (fluxing agent, aluminium oxide and phosphates). We observed that the amounts of fluxing agents needed to inhibit the crystallization prevent effective foaming and were thus decreased. Decreasing the content of the fluxing agent resulted in samples with a lower density. We found that adding phosphates to the foaming mixtures decreases the crystalline content, open porosity and thermal conductivity of the foamed glass, samples became less crystalline with the presence of the devitrite phase only. Obtained foamed glass samples had a thermal conductivity ranging from 57 to 66 mW m^{-1}K^{-1}. Additionally, crystallization can be inhibited with the addition of water glass, obtaining samples with thermal conductivity ranging from 57 to 59 mW m^{-1}K^{-1}. In the second part of our research, we investigated the possibility to use flat-glass waste in foamed glass production. Preliminary results are promising due to the higher glass stability towards crystallization. The obtained foamed glass samples are less crystalline, with one dominant crystalline phase, devitrite phase. Interestingly, flat glass-based foamed glass exhibits a very closed porous structure (closed porosity up to 96%).

The use of water glass affects the environmental impact of foamed glass production while maintaining high-quality products characterized by a low thermal conductivity. To further explain this effect and understand the role of the water, we investigated the foaming ability of hydrothermally treated glass powder. For this purpose, we used three types of waste glass (cathode-ray-tube glass – CRT, flat glass and mixed color bottle glass) and hydrothermally treated them with different water contents. The susceptibility of glass to bond water molecules within its structure affected the decrease of foaming temperature and increased expansion. CRT glass hydrothermally treated with 30 wt.% of water resulted in a foamed glass sample with the lowest density ($\sim$ 320 kg m^{-3}). Similarly, as with water glass, the expansion mechanism is likely related to the formation of carbonates which decompose later during the heating of the hydrothermally treated powder. Interestingly, an XRD analysis of hydrothermally treated glass powders suggests the presence of zeolites that disappear after the heat treatment. Additionally, **hydrothermally treated glass powder can be used in combination with a carbonaceous foaming agent**, where the inhibition of the reaction between the atmosphere and carbon, **allows the implementation of such a process in the air**. Future research will be focused on the practical use of hydrated glass (water glass and/or hydrothermally treated glass powders) and newly revealed crystallization mechanisms, for the sustainable production of foamed glass.
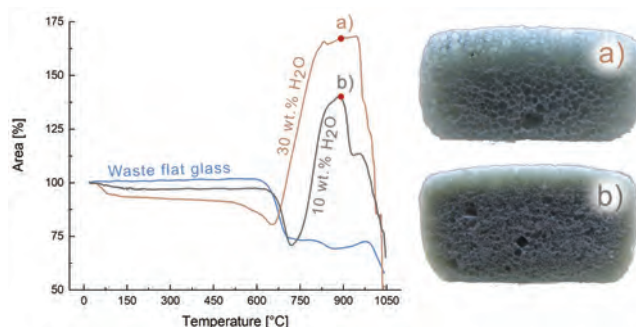
Figure 7: Expansion of the samples (in area %) as a function of temperature.

Some outstanding publications in the past year

1. Maček, Marjeta, Daneu, Nina, Čontala, Alja, Santra, Saswati, Mohaideen, Kamal Khaja, Likozar, Blaž, Spreitzer, Matjaž. SrTiO3/Bi4Ti3O12 nanoheterostructural platelets synthesized by topotactic epitaxy as effective noble-metal-free photocatalysts for pH-neutral hydrogen evolution. *ACS applied materials & interfaces*, ISSN 1944-8244, 2021, vol. 13, no. 1, str. 370-381, doi: 10.1021/acsami.0c16253. [COBISS.SI-ID 45083139]

2. Hribar, Uroš, Spreitzer, Matjaž, Koenig, Jakob. Applicability of water glass for the transfer of the glass-foaming process from controlled to air atmosphere. *Journal of cleaner production*, ISSN 0959-6526. [Print ed.], 2021, vol. 282, str. 125428-1-125428-12, doi: 10.1016/j.jclepro.2020.125428. [COBISS.SI-ID 45373443]

3. Golobič, Amalija, Meden, Anton, Spreitzer, Matjaž, Škapin, Srečo D.. Phase equilibria and microwave dielectric properties in the ternary La2O3–TiO2–Nb2O5 system. *Journal of the European ceramic society*, ISSN 0955-2219. [Print ed.], 2021, vol. 41, no. 14, str. 7035-7043, doi: 10.1016/j.jeurceramsoc.2021.07.046. [COBISS.SI-ID 79493379]

4. Smiljanić, Sonja V., Hribar, Uroš, Spreitzer, Matjaž, Koenig, Jakob. Influence of additives on the crystallization and thermal conductivity of container glass cullet for foamed glass preparation. *Ceramics international*, ISSN 0272-8842. [Print ed.], 2021, vol. 47, iss. 23, str. 32867-32873, tabele, graf. prikazi, doi: 10.1016/j.ceramint.2021.08.183. [COBISS.SI-ID 79486723]

5. Vukomanović, Marija, Mar Cendra, Maria Del, Baelo, Aida, Torrents, Eduard. Nano-engineering stable contact-based antimicrobials : chemistry at the interface between nano-gold and bacteria. *Colloids and surfaces. B, Biointerfaces*, ISSN 0927-7765. [Print ed.], 2021, vol. 208, str. 112083-1-112083-11, doi: 10.1016/j.colsurfb.2021.112083. [COBISS.SI-ID 75597571]

Awards and Appointments

1. Alja Čontala, 13th Jožef Stefan IPSS Conference and 15th CMBE Day, Greenest Research Award.
2. Matjaž Spreitzer, Srečo Škapin: Silver award of the CCIS for the innovation Green Energy from aluminium waste, Maribor, Chamber of Commerce and Industry of Slovenia.

Organization of conferences, congresses and meetings

1. Workshop on international project M.ERA-NET "SunToChem: Engineering of perovskite photocatalysts for sunlight-driven hydrogen evolution from water splitting", 15. 6. 2021 in 3. 12. 2021 (virtual).
2. Symposium co-organization: Advances in Dielectric Materials and Electronic Devices, MS & T21- Materials Science and Technology, Columbus, Ohio, USA, 17.–20. 10. 2021 (virtual).
3. Kick-off meeting of the international project H2020 INNOSUP-01-2020: "Advanced Materials & manufacturing technologies United for LightwEighT - AMULET", 6. 9. 2021 (virtual).
4. Symposium co-organization S5: Mesoscale Phenomena in Ferroic Nanostructures: From Patterns to Functionalities, EMA 2021 - Meeting on electronic materials and applications, 19.–21. 1. 2021 (virtual).
5. Workshop on international project ERAMIN2 "ANTISOLVO: Antisolvent precipitation to extract the value from end-of-life Nd-Fe-B magnets", 14. 1. 2021 (virtual).

INTERNATIONAL PROJECTS

1. Investigation of NdDyCoCuFe Rare Earth Alloys Alloys and Related Compounds
   Prof. Matjaž Spreitzer
   Urban Mining Company
2. KET4CLEAN-INNOWEAR-TEX; Costs of Work of K9 on the Case KET4CLEAN PRODUCTION-INNOWEAR-TEX
   Prof. Matjaž Spreitzer
   Innowear-tex Kft.
3. COST CA 17140; Cancer Nanomedicine - From the Bench to the Bedside (NANO2CL)
   Marija Vukomanović
   Cost Association Aisbl
4. Stay of Nina Kuzmić in Oulu, Finland - Low Temperature Densification of Strontium Titanate Ceramics, May - June 2020
   Nina Kuzmić
   Jecs Trust
5. COST CA20116; OPERA - European Network for Innovative and Advanced Epitaxy
   Prof. Matjaž Spreitzer
   Cost Association Aisbl
6. H2020 - AMULET; Advanced Materials and Manufacturing Technologies united for LightwEight
   Dr. Jakob König
   European Commission
7. Stoichiometry Engineering of Epitaxial PMN-PT Thin Films
   Prof. Matjaž Spreitzer
   Slovenian Research Agency

RESEARCH PROGRAMMES

1. Advanced inorganic magnetic and semiconducting materials
   Prof. Mihael Drofenik
2. Contemporary Inorganic Materials and Nanotechnologies
   Prof. Matjaž Spreitzer

R & D GRANTS AND CONTRACTS

1. Non-traditional isotopes as identifiers of authigenic carbonates
   Prof. Srečo Davor Škapin
2. Synthesis and characterization of alkali activated foams based on different waste
   Prof. Srečo Davor Škapin
3. Model system based interface design for enhancement of the electrochemical performance of Ni-rich NMC for Li-ion batteries
   Prof. Matjaž Spreitzer
4. Subglacial carbonate deposits - a new source for studying the presence of glaciers in a glaciokarstic environment
   Prof. Srečo Davor Škapin
5. Nanoscale investigations of diffusion controlled topotaxial phase transformations in rutile-corundum host systems
   Asst. Prof. Nina Daneu
6. Engineering of oxides on silicon for future electronics
   Prof. Matjaž Spreitzer

7. Mineral inclusions in garnet from macroscopic to atomic scale: Opening the petrogenetic archive
   Asst. Prof. Nina Daneu
8. Strain and domain structure engineering in epitaxial relaxor ferroelectric thin films
   Prof. Matjaž Spreitzer
9. Mechano-chromic, voltage-sensitive electrostimulators: innovative piezoelectric biomaterials for electro-stimulated cellular growth
   Marija Vukomanović
10. Engineering of relaxor ferroelectric thin films for piezoelectric and energy storage applications
    Prof. Matjaž Spreitzer
11. Photoelektrochemical Hydrogen Evolution from Graphene Oxide Enabled Epitaxial Silicon-Oxide Heterostructures
    Prof. Matjaž Spreitzer
12. Semiconductor - dielectric heterostructures for photoelectrochemical hydrogen evolution, SeDiHe
    Prof. Matjaž Spreitzer
13. Extended defects in natural and synthesized perovskite oxides: nanogeochemcial indicators and functional interfaces
    Asst. Prof. Nina Daneu
14. Applicability of the cold sintering process to clay minerals
    Prof. Srečo Davor Škapin
15. Multiscale modeling of photocatalytic CO2 reduction with computer intensive simulations
    Dr. Marjeta Maček Kržmanc
16. Innovative procedures for advanced surface properties of medical stainless steel
    Marija Vukomanović
17. Mineral wool composite with improved insulation properties
    Dr. Jakob König
18. Innovative ECO plasma seed treatment (for sowing and for human and animal diet/nutrition
    Marija Vukomanović
    Ministry of Education, Science and Sport
19. Control of crystallization in glass materials for thermal insulation
    Dr. Sonja Smiljanić
    Ministry of Education, Science and Sport
20. ANTISOLVO - Antisolvent precipitation to extract the value from end-of-life Nd-Fe-B magnets
    Prof. Srečo Davor Škapin
    Ministry of Education, Science and Sport
21. XRD Analysis
    Prof. Matjaž Spreitzer

NEW CONTRACTS

1. Mineral wool composite with improved insulation properties
   Dr. Jakob König
   Knauf Insulation, d. o. o., Škofja Loka
2. Determination of potential structural changes of proteins using the following analytical techniques: UV-Vis-NIR spectrometry, fluorescence spectrometry, X-ray diffraction and circular dichroism
   Prof. Matjaž Spreitzer
   Lek d. d.

VISITORS FROM ABROAD

1. Dr Taisia Alifirova, Department of Lithospheric Research, University of Vienna, Vienna, Austria, 30. 8.–5. 9. 2021.
2. Dr Arjen Steiner, Schaumglas Global Consulting GmbH (SGGC), Gelsenkirchen, Germany, 30. 9. 2021.
3. Dr Sonja Jovanovič, Dr Zoran Jovanović, Vinča Nuclear Research Institute, Belgrade, Serbia, 12.–18. 5. 2021.
4. Dr Federico Baiutti, Catalonia Institute for Energy Research, Barcelona, Spain, 27.–30. 9. 2021.
5. Prof. dr. Gertjan Koster, University of Twente, Enshede, Netherlands, 14.–20. 11. 2021.
6. Dr Manal Benyoussef, Laboratoire de Physique de la Matière Condensée (LPMC), Amiens, France, 19. 12. 2021–21. 1. 2022.
7. Dr Jamal Belhadi, Laboratoire de Physique de la Matière Condensée (LPMC), Amiens, France, 19. 12. 2021–21. 1. 2022.

Visiting Researchers
1. Dr Mihaela Apetrei, Department of Chemistry, Akdeniz University, Antalya, Turkey, 4. 1. 2021–3. 1. 2022.
2. Dr Suraj Gupta, School of Engineering, University of Liverpool, United Kingdom, 21. 6. 2021–20. 6. 2023.
3. Dr Hsin-Chia Ho, National Taiwan University, Taipei City, Taiwan, 7. 6. 2021–6. 6. 2023.
4. Dr Sonja Smiljanić, Univerzitet u Beogradu, Tehnološko-metalurški fakultet, Belgrade, Serbia, 1. 6. 2019–31.3. 2022.

STAFF

Researchers
1. Asst. Prof. Nina Daneu
2. Dr. Suraj Gupta
3. Dr. Heli Maarit Jantunen
4. Dr. Jakob König
5. Dr. Gertjan Koster
6. Dr. Špela Kunej
7. Dr. Marjeta Maček Kržmanc
8. **Prof. Matjaž Spreitzer, Head**
9. Prof. Srečo Davor Škapin
10. Dr. Marija Vukomanović

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ORIGINAL ARTICLE

1. Marjeta Maček Kržmanc, Nina Daneu, Alja Čontala, Saswati Santra, Kamal Khaja Mohaideen, Blaž Likozar, Matjaž Spreitzer, "SrTiO$_3$/Bi$_4$Ti$_3$O$_{12}$ nanoheterostructural platelets synthesized by topotactic epitaxy as effective noble-metal-free photocatalysts for pH-neutral hydrogen evolution", *ACS applied materials & interfaces*, 2021, **13**, 1, 370-381.

2. Martina Kocijan *et al.* (11 authors), "Graphene-based TiO$_2$ nanocomposite for photocatalytic degradation of dyes in aqueous solution under solar-like radiation", *Applied sciences*, 2021, **11**, 9, 3966.

3. Roxana-Mihaela Apetrei, Pinar Camurlu, "Facile copper-based nanofibrous matrix for glucose sensing: Enzymatic vs. non-enzymatic", *Bioelectrochemistry*, 2021, **140**, 107751.

4. Martina Kocijan, Lidija Ćurković, Tina Radošević, Matejka Podlogar, "Enhanced photocatalytic activity of hybrid r*G*O@TiO$_2$/CN nanocomposite for organic pollutant degradation under solar light irradiation", *Catalysts*, 2021, **11**, 9, 1023.

5. Hitoshi Ohsato, Jobin Varghese, Akinori Kan, Jeong Seog Kim, Isao Kagomiya, Hirotaka Ogawa, Mailadil T. Sebastian, Heli Jantunen, "Volume crystallization and microwave dielectric properties of indialite/ cordierite glass by TiO$_2$ addition", *Ceramics international*, 2021, **47**, 2, 2735-2742.

6. Rasmus R. Petersen, Jakob Koenig, Niels Iversen, Martin B. Østergaard, Yuanzheng Yue, "The foaming mechanism of glass foams prepared from the mixture of Mn$_3$O$_4$, carbon and CRT panel glass", *Ceramics international*, 2021, **47**, 2, 2839-2847.

7. Damjan Vengust, Boštjan Jančar, Tilen Sever, Andreja Šestan, Vid Bobnar, Zdravko Kutnjak, Nina Daneu, Danilo Suvorov, Matjaž Spreitzer, "Improved environmental stability of thermoelectric ceramics based on intergrowths of Ca$_3$Co$_4$O$_9$ − Na$_{0.75}$CoO$_2$", *Ceramics international*, 2021, **47**, 8, 11687-11693.

8. Katja Traven, Mark Češnovar, Srečo D. Škapin, Vilma Ducman, "High temperature resistant fly-ash and metakaolin-based alkali-activated foams", *Ceramics international*, 2021, **47**, 17, 25105-25120.

9. Manal Benyoussef, Moneim Zannen, Jamal Belhadi, Bouchaib Manoun, Zdravko Kutnjak, Damjan Vengust, Matjaž Spreitzer, Mimoun El Marssi, Abdelilah Lahmar, "Structural, dielectric, and ferroelectric properties of Na$_{0.5}$(Bi$_{1-x}$Nd$_x$)$_{0.5}$TiO$_3$ ceramics for energy storage and electrocaloric application", *Ceramics international*, 2021, **47**, 18, 26539-26551.

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11. Sonja V. Smiljanić, Uroš Hribar, Matjaž Spreitzer, Jakob Koenig, "Influence of additives on the crystallization and thermal conductivity of container glass cullet for foamed glass preparation", *Ceramics international*, 2021, **47**, 23, 32867-32873.

12. Laura Moya-Andérico, Marija Vukomanović, Maria del Mar Cendra, Miriam Segura-Feliu, Vanessa Gil, José A. del Rio, Eduard Torrents, "Utility of *Galleria mellonella* larvae for evaluating nanoparticle toxicology", *Chemosphere*, 2021, **266**, 129235.

13. Marija Vukomanović, Maria del Mar Cendra, Aida Baelo, Eduard Torrents, "Nano-engineering stable contact-based antimicrobials: chemistry at the interface between nano-gold and bacteria", *Colloids and surfaces. B, Biointerfaces*, 2021, **208**, 112083.

14. Paula Cimavilla-Roman, Juan Villafañe-Calvo, Alberto Lopez-Gil, Jakob Koenig, Miguel A. Rodriguez-Perez, "Modelling of the mechanisms of heat transfer in recycled glass foams", *Construction & building materials*, 2021, **274**, 122000.

15. Zouhair Hanani *et al.* (14 authors), "Morphogenesis mechanisms in the hydrothermal growth of lead-free BCZT nanostructured multipods", *CrystEngComm*, 2021, **23**, 30, 5249-5256.

16. Nina Kuzmić, Srečo D. Škapin, Mikko Nelo, Heli Jantunen, Matjaž Spreitzer, "Dielectric properties of upside-down SrTiO$_3$/Li$_2$MoO$_4$ composites fabricated at room temperature", *Frontiers in materials*, 2021, **8**, 669421.

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22. Ayhan Altun, Roxana-Mihaela Apetrei, Pinar Camurlu, "Reagentless amperometric glucose biosensors: ferrocene-tethering and copolymerization", *Journal of the Electrochemical Society*, 2021, **167**, 10, 107507.

23. Amalija Golobič, Anton Meden, Matjaž Spreitzer, Srečo D. Škapin, "Phase equilibria and microwave dielectric properties in the ternary La$_2$O$_3$ − TiO$_2$ − Nb$_2$O$_5$ system", *Journal of the European ceramic society*, 2021, **41**, 14, 7035-7043.

24. Miha Škarabot, Marjeta Maček Kržmanc, Lina Rupnik, Gojmir Lahajnar, Danilo Suvorov, Igor Muševič, "Electric-field-induced reorientation of ferroelectric micro- and nano-platelets in the nematic liquid crystal", *Liquid crystals*, 2021, **48**, 3, 385-394.

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28. Petra S. Pálvölgyi *et al.* (12 authors), "Lightweight porous silica foams with extreme-low dielectric permittivity and loss for future 6G wireless communication technologies", *Nano research*, 2021, **14**, 1450-1456.

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32. Peter Baláž, Emmanuel Guilmeau, Marcela Achimovičová, Matej Baláž, Nina Daneu, Oleksandr Dobrozhan, Mária Kaňuchova, "Bismuth doping in nanostructured tetrahedrite: scalable synthesis and thermoelectric performance", *Nanomaterials*, 2021, **11**, 6, 1386.

33. Matjaž Kristl, Sašo Gyergyek, Srečo D. Škapin, Janja Kristl, "Solvent-free mechanochemical synthesis and characterization of nickel tellurides with various stoichiometries: NiTe, $NiTe_2$ and Ni_2Te_3", *Nanomaterials*, 2021, **11**, 8, 1959.

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38. Anna Motorzhina *et al.* (13 authors), "Innovative gold/cobalt ferrite nanocomposite: physicochemical and cytotoxicity properties", *Processes*, 2021, **9**, 12, 2264.

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46. Damir Dominko *et al.* (11 authors), "Single crystal-like thin films of blue bronze", *Thin solid films*, 2021, **731**, 138745.

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REVIEW ARTICLE

1. Matjaž Spreitzer *et al.* (17 authors), "Epitaxial ferroelectric oxides on silicon with perspectives for future device applications", *APL materials*, 2021, **9**, 4, 040701.

2. Mladenika Malenica *et al.* (17 authors), "Perspectives of microscopy methods for morphology characterisation of extracellular vesicles from human biofluids", *Biomedicines*, 2021, **9**, 6, 603.

3. Jiandong Liu *et al.* (51 authors), "2021 Roadmap: electrocatalysts for green catalytic processes", *JPhys materials*, 2021, **4**, 2, 022004.

PUBLISHED CONFERENCE CONTRIBUTION

1. Tomaž Lutman, Marija Vukomanović, "Towards the market: novel antimicrobial material", In: *IS 2021, 14th International Technology Transfer Conference, 7. October 2021, Ljubljana, Slovenia*, Proceedings of the 24th International Multiconference Information Society, volume E, Institut "Jožef Stefan", 2021, 57-61.

2. Patrick Seleš, Žiga Lipovšek, Martina Kocijan, Tina Radošević, Damjan Vengust, Matejka Podlogar, "Synthesis of ZnO powders with different morphologies for photocatalytic degradation", In: *56th International Conference on Microelectronics, Devices and Materials & the Workshop on Personal Sensors for Remote Health Care Monitoring, 22-24 September 2021, Ljubljana, Slovenia*, Proceedings, MIDEM, 2021, 35-42.

THESES AND MENTORING

1. Tjaša Parkelj Potočnik, *Surfaces and interfaces in the growth of $SrTiO_3$ on Si by pulsed laser deposition:* doctoral dissertation, Ljubljana, 2021 (mentor Matjaž Spreitzer).

2. Sara Tominc, *Charge compensation mechanisms and twinning in doped SnO_2-based ceramics:* doctoral dissertation, Ljubljana, 2021 (mentor Aleksander Rečnik; co-mentor Nina Daneu).

DEPARTMENT OF BIOCHEMISTRY, MOLECULAR AND STRUCTURAL BIOLOGY B-1

The research activities of the members of the B1 department are largely focused on studies of the physiological role of proteases and their endogenous protein inhibitors in normal and pathological states. The studies involve the mechanisms of protease action and the structural and functional properties of proteases and their inhibitors, as well as some other enzymes. Molecular mechanisms of protease action and regulation are only partially understood; therefore, a lot of work, especially to find more physiological substrates and the signalling pathways they regulate, remains to be done.

Protease research has undergone a major expansion in the past decade, largely due to the extremely rapid development of new technologies, such as quantitative proteomics and *in vivo* imaging, as well as the extensive use of *in vivo* models. These have led to the identification of physiological substrates and resulted in a paradigm shift from the concept of proteases as protein-degrading enzymes to proteases as key signalling molecules. Their catalytic activities are precisely regulated, the most important ways being zymogen activation and inhibition by their endogenous protein inhibitors. Any imbalance in the regulation of proteases can lead to pathologies, such as autoimmune, cardiovascular, neurologic and neurodegenerative disorders, as well as cancer. Thus, proteases represent an extremely important group of targets for therapeutic intervention.

Head:
Prof. Boris Turk

In the continuation of our research on the physiological roles of proteases, we investigated the role of the high-temperature requirement A (HtrA) protease secreted by the group 1 carcinogen *Helicobacter pylori*. Since the intact gastric epithelium is the primary target for *H. pylori* in the stomach, we aimed to identify the HtrA substrates on the cell surface of gastric cells. In this study we treated human gastric epithelial cells with recombinant HtrA and used LC–MS/MS to identify the membrane proteins released from the cell surface. We identified several extracellular membrane targets including desmoglein-2 (Dsg2), since Dsg2 is a component of desmosomal junctions and highly expressed in epithelial cells and cardiomyocytes. We therefore propose that Dsg2 cleavage by HtrA contributes to the disintegration of the gastric epithelial barrier in response to *H. pylori* infections (Bernegger et al., 2021). This research is part of a collaboration with prof. Silja Wessler (UNI Salzburg).

In collaboration with prof. Peter Hamar (Semmelweis University, Hungary) we have investigated the molecular changes elicited by modulated electro-hyperthermia (mEHT) using multiplex methods in an aggressive, therapy-resistant triple-negative breast-cancer model. In mEHT, a focused electromagnetic field is generated within the tumour, inducing cell death by thermal and nonthermal effects. With next-generation sequencing, nanostring and mass spectrometry we identified that mEHT induced the upregulation of the stress-related Hsp70 and cleaved caspase-3 proteins, resulting in the effective inhibition of tumour growth and proliferation. In addition, several acute stress-response proteins, including protease inhibitors, coagulation and heat-shock factors, and complement family members were among the most upregulated treatment-related genes/proteins. We also confirmed that the heat-shock factor inhibitor KRIBB11 reduced mEHT-induced complement factor 4 mRNA increase, indicating that the inhibition of this stress response is likely to enhance the effectiveness of mEHT and other cancer treatments (Schvarcz et al., 2021).

Figure 1: X-ray screening of drug-repurposing libraries reveals compound binding sites distributed across the complete M^pro surface. (**A**) Schematic drawing of M^pro dimer structure. Protomer A in white, protomer B in red. For clarity, the 29 binding compounds (yellow sticks) are only depicted on one of the two protomers. Catalytic residues H41 and Cys145, active site and two allosteric drug binding sites are highlighted. (**B**) Close-up view of active site with peptide substrate bound (blue sticks), modelled after SARS-CoV M^pro (PDB 2Q6G). The scissile bond is indicated in yellow and with a green arrow. Substrate binding pockets S1', S1, S2 and S4 are indicated by colours.

Our research on the endogenous inhibitors of proteases was primarily focused on inhibitors of cathepsins, stefins and cystatins. We thus explored the role of cystatin C, the major extracellular cathepsin inhibitor, in inflammation and sepsis (Biasizzo et al., 2021, Cells). We demonstrated that cystatin C-deficient mice (CstC KO) were significantly more sensitive to the lethal LPS-induced sepsis. We further showed increased caspase-11 gene expression and the enhanced processing of pro-inflammatory cytokines IL-1β and IL-18 in CstC KO bone-marrow-derived macrophages (BMDM) upon LPS and ATP stimulation. The pre-treatment of BMDMs with the cysteine cathepsin inhibitor E-64d did not reverse the effect of CstC deficiency on IL-1β processing and secretion, suggesting that the increased cysteine cathepsin activity determined in CstC KO BMDMs is not essential for NLRP3 inflammasome activation. The CstC deficiency had no effect on (mitochondrial) reactive oxygen species (ROS) generation, the MAPK signalling pathway or the secretion of anti-inflammatory cytokine IL-10. However, CstC-deficient BMDMs showed dysfunctional

autophagy, as autophagy induction via mTOR and AMPK signalling pathways was suppressed and the accumulation of SQSTM1/p62 indicated a reduced autophagic flux. Our study demonstrates that the excessive inflammatory response to the LPS-induced sepsis in CstC KO mice is dependent on increased caspase-11 expression and impaired autophagy.

Stefin B (cystatin B) is the major intracellular inhibitor of cathepsins, and the loss-of-function mutations in the stefin B gene were reported in patients with Unverricht–Lundborg disease (EPM1), a form of progressive myoclonus epilepsy. Stefin B-deficient mice, a mouse model of the disease, display key features of EPM1. Although the underlying mechanism is not yet completely clear, it was reported that the impaired redox homeostasis and inflammation in the brain contribute to the progression of the disease. In a study (Trstenjak et al., 2021, Antioxidants) we investigated

*Figure 2: Covalent and non-covalent binders in the active site of M^{pro}. Bound compounds are depicted as coloured sticks while the surface of M^{pro} is shown in grey with selected interacting residues as sticks. Substrate binding pockets are coloured as in Figure 1. Hydrogen bonds are depicted by dashed lines. (**A**) tolperisone, (**B**) HEAT, (**C**) isofloxythepin, (**D**) triglycidyl isocyanurate, (**E**) calpeptin, (**F**) MUT056399.*

whether lipopolysaccharide (LPS)-triggered neuroinflammation affected the protein levels of redox-sensitive proteins: thioredoxin (Trx1), thioredoxin reductase (TrxR), peroxiredoxins (Prxs) in brain and cerebella of stefin B-deficient mice. LPS challenge was found to result in a marked elevation of Trx1 and TrxR in the brain and cerebella of stefin B deficient mice, while Prx1 was upregulated only in cerebella after LPS challenge. Mitochondrial peroxiredoxin 3 (Prx3), was upregulated also in the cerebellar tissue lysates prepared from unchallenged stefin B-deficient mice, while after LPS challenge Prx3 was upregulated in stefin B-deficient brain and cerebella. Our results indicate the important role of oxidative stress in the progression of the disease. In addition, we also performed studies on the structure and folding of stefin B, which has been used as a model protein. In the last year we have continued to study the role of polyphenolic anti-oxidants on protein aggregation and have observed the synergy of the inhibitory action of some polyphenols including curcumin and quercetin and vitamin C (vitC) (Jahić Mujkić et al., 2021, Antioxidants). In an overview, E. Žerovnik (Žerovnik E, 2021, Front. Chem.) discussed the common traits between amyloid-forming proteins and known pore-forming proteins, including viroporins. Further along these lines together with collaborators from NIC (prof. Novič's group) we have searched machine-learning methods to predict the transmembrane

regions and ganglioside binding sites in amyloid-forming proteins (Venko et al., 2021, Front. Mol. Neurosci). A set of 30 amyloid-forming proteins was used as the database. A range of amino-acid sequence tools were then applied, in order to predict AP domains and provide context on future experiments that are needed to contribute towards a deeper understanding of amyloid toxicity, which fitted well with the known experimental data.

The crucial work of our department was undoubtedly a huge collaboration on understanding the molecular features of the SARS-CoV-2 main protease, a key drug target of the virus as one of the two viral proteases essential to yield functional viral proteins (Günther et al., Turk D., 2021) published in Science. Screening of more than 5000 compounds that are either approved drugs or drugs in clinical trials resulted in several crystal structures of the active site and allosteric inhibitors of the SARS-CoV-2 main protease. The most potent inhibitor, calpeptin, binds covalently in the active site, whereas the second-most potent, pelitinib, binds at an allosteric site. Calpeptin dual targeting of cathepsins and Mpro is also explored as an important path for the therapeutical inhibition of SARS-CoV-2. This was also the very first work published on SARS-CoV-2 virus from Slovenia.

Tušar et al. (2021, Int J Mol Sci) wrote a review analysing the mechanisms of inhibition of cysteine proteases on the basis of structural information and compiled kinetic data. It reveals that the protein fold is not a major obstacle to the evolution of a protease inhibitor and that there appears to be no general rule governing the inhibitory mechanism. However, the analysis suggests that the shape of the active site cleft of proteases imposes some restraints, mainly based on the shape and solvent exposure of the S1 binding site. While the pocket-shaped S1 binding site buried in the structure of the protease enables substrate-like binding mechanisms of inhibitors, with the S1 binding site in part exposed to a solvent, the substrate-like inhibition cannot be employed. Except for papain-like proteases, all proteases appear to belong to the first group of proteases.

The novel finding that cathepsin X is a dimeric protein (Dolenc et al., 2021, BBA Proteins Proteom.) opens new horizons in the understanding of its function and the underlying pathophysiological mechanisms of various diseases, including neurodegenerative disorders in humans. Namely, human cathepsin X is an exopeptidase belonging to the cathepsin family of 11 lysosomal cysteine proteases. We expressed recombinant procathepsin X in *Pichia pastoris* and *in vitro* cleaved it into its active, mature form using aspartic cathepsin E. We found, using size-exclusion chromatography, X-ray crystallography, and small-angle X-ray scattering, that cathepsin X is biologically active as a homodimer with a molecular weight of ~53 kDa.

In addition, we collaborated with other research groups from Slovenia and several foreign countries (Germany, Austria, Hungary, Switzerland, Croatia, Poland, United Kingdom, Netherlands, Japan and USA).

Some outstanding publications in the past year

1. Biasizzo M, Trstenjak-Prebanda M, Dolinar K, Pirkmajer S, Završnik J, Turk B, Kopitar-Jerala N. Cystatin C Deficiency Increases LPS-Induced Sepsis and NLRP3 Inflammasome Activation in Mice. Cells. 2021. doi: 10.3390/cells10082071.
2. Jahić Mujkić A, Tušek Žnidarič M, Berbić S, Žerovnik E. Synergy of the Inhibitory Action of Polyphenols Plus Vitamin C on Amyloid Fibril Formation: Case Study of Human Stefin B. Antioxidants (Basel). 2021. doi: 10.3390/antiox10091471.
3. Bernegger S, Vidmar R, Fonovic M, Posselt G, Turk B, Wessler S. Identification of Desmoglein-2 as a novel target of Helicobacter pylori HtrA in epithelial cells. Cell Commun Signal. 2021. doi: 10.1186/s12964-021-00788-x.
4. Günther et al., X-ray screening identifies active site and allosteric inhibitors of SARS-CoV-2 main protease. Science. 2021. doi: 10.1126/science.abf7945.
5. Dolenc I, Štefe I, Turk D, Taler-Verčič A, Turk B, Turk V, Stoka V. Human cathepsin X/Z is a biologically active homodimer. Biochim Biophys Acta Proteins Proteom. 2021. doi: 10.1016/j.bbapap.2020.140567.

Awards and Appointments

1. Monika Biasizzo: Young Investigator Award Nomination: Best Speaker at 38th Winter School on proteinases and their inhibitors, ASBMB virtual conference, Impaired autophagy and increased susceptibility to LPS-induced sepsis in cystatin C-deficient mice.
2. Eva Vidak: Young Investigator Award Nomination: Best Speaker at 38th Winter School on proteinases and their inhibitors, ASBMB virtual conference, Identification of extracellular substrates of caspases 3, 7, and 1.

Organization of conferences, congresses and meetings

1. 38th Winter School on proteinases and their inhibitors, ASBMB virtual conference, 24– 26 February 2021 (virtual), co-organiser.

Patent granted

1. Stephen James Moore, Margaret Thy Luu Hyugen, Daniel Robert Hostetter, Olga Vasiljeva, Jason Gary Sagert, Jonathan Alexander Terrett, James William West, Matrix metalloprotease-cleavable and serine protease-cleavable substrates and methods of use thereof, US11046759 (B2), US Patent Office, 29. 06. 2021.

INTERNATIONAL PROJECTS

1. EFSA - EU-FORA; Implementation of Matrix Effects into Chemical Food Contaminant Risk Assessment
Asst. Prof. Livija Tušar
European Food Safety Authority - EFSA
2. The Role of Cystatins in Neuroinflamamtion
Prof. Nataša Kopitar – Jerala
Slovenian Research Agency
3. Innovative ECO plasma seed treatment (for sowing and for human and animal diet/nutrition
Prof. Boris Turk
Ministry of Education, Science and Sport

RESEARCH PROGRAMMES

1. Structural biology
Prof. Dušan Turk
2. Proteolysis and its regulation
Prof. Boris Turk

R & D GRANTS AND CONTRACTS

1. Molecular genetic biomarkers and mechanisms of unresponsiveness to biological therapyanti-TNF in patients with chronic immune diseases
Prof. Boris Turk
2. Structural insight into the mechanism of Clostridium difficle surface formation
Prof. Dušan Turk

3. Cathepsins B and X in breast cancer stem cells – molecular targets and relevance for antitumor therapy
Prof. Marko Fonović
4. Aptamers and hydrodynamic cavitation, an accessible tool for the analysis of organic residuals in archaeological pottery
Prof. Marko Fonović
5. Role of legumain in infection and inflammation
Prof. Marko Fonović
6. Role of cysteine cathepsins in complement activation in cancer
Prof. Boris Turk
7. Mineral inclusions in garnet from macroscopic to atomic scale: Opening the petrogenetic archive
Prof. Boris Turk
8. Cathepsin-based non-invasive diagnostics and theranostics of cancer
Prof. Boris Turk
9. Human cathepsin F: An unusual cysteine protease involved in neurodegeneration
Prof. Veronika Stoka
10. Dissecting cancer activome to develop new generation of antibody-drug conjugates
Prof. Boris Turk
11. Systemic determination of legumain physiological roles
Prof. Marko Fonović

NEW CONTRACTS

1. Determination of protein concentration by Bradford methodology
Prof. Marko Fonović
Lek d. d.
2. Proteomic analysis
Prof. Marko Fonović

STAFF

Researchers
1. Dr. Iztok Dolenc
2. Prof. Marko Fonović
3. Prof. Nataša Kopitar - Jerala
4. Prof. Brigita Lenarčič*
5. Prof. Veronika Stoka
6. Dr. Andrej Šali
7. **Prof. Boris Turk, Head**
8. Prof. Dušan Turk
9. Asst. Prof. Livija Tušar
10. Prof. Olga Vasiljeva
11. Prof. Eva Žerovnik

Postdoctoral associates
12. *Dr. Janja Božič, left 01.09.21*
13. Dr. Katarina Karničar
14. Dr. Nežka Kavčič
15. Dr. Andreja Kozak
16. Dr. Nataša Lindič
17. Dr. Georgy Mikhaylov
18. Dr. Jure Pražnikar*
19. Dr. Aleksandra Usenik
20. Dr. Robert Vidmar

Postgraduates
21. Monika Biasizzo, B. Sc.
22. Ana Ercegovič Rot, B. Sc.

23. Marija Grozdanić, M. Sc.
24. Urban Javoršek, B. Sc.
25. Matej Kolarič, B. Sc.
26. Jure Loboda, B. Sc.
27. Petra Matjan Štefin, B. Sc.
28. Matej Novak, B. Sc.
29. Tilen Sever, B. Sc.
30. Tea Sinožić, M. Sc.
31. Mojca Trstenjak Prebanda, B. Sc.
32. Eva Vidak, B. Sc.
33. Miki Zarić, B. Sc.
34. Viktor Zupančič, B. Sc.

Technical officers
35. Marinka Horvat, B. Sc.
36. Maja Orehek, B. Sc.
37. Tjaša Peternel, B. Sc.
38. Andreja Sekirnik, B. Sc.
39. Ivica Štefe, B. Sc.

Technical and administrative staff
40. Dejan Pelko
41. Polonca Pirš

Note:
* part-time JSI member

BIBLIOGRAPHY

ORIGINAL ARTICLE

1. Mojca Trstenjak-Prebanda, Petra Matjan-Štefin, Boris Turk, Nataša Kopitar-Jerala, "Altered expression of peroxiredoxins in mouse model of progressive myoclonus epilepsy upon LPS-induced neuroinflammation", *Antioxidants*, 2021, **10**, 3, 357.
2. Alma Jahić Mujkić, Magda Tušek-Žnidarič, Selma Berbić, Eva Žerovnik, "Synergy of the inhibitory action of polyphenols plus vitamin C on amyloid fibril formation: case study of human stefin B", *Antioxidants*, 2021, **10**, 9, 1471.
3. Iztok Dolenc, Ivica Klemenčič, Dušan Turk, Ajda Taler-Verčič, Boris Turk, Vito Turk, Veronika Stoka, "Human cathepsin X/Z is a biologically active homodimer", *Biochimica et biophysica acta. Proteins and proteomics.*, 2021, **1869**, 2, 140567.
4. Hikmat H. Assi *et al.* (27 authors), "Conditional PD-1/PD-L1 probody therapeutics induce comparable antitumor immunity but reduced systemic toxicity compared with traditional anti–PD-1/PD-L1 agents", *Cancer immunology research*, 2021, **9**, 12, 1451-1464.
5. Csaba András Schvarcz *et al.* (14 authors), "Modulated electro-hyperthermia induces a prominent local stress response and growth inhibition in mouse breast cancer isografts", *Cancers*, 2021, **13**, 7, 1744.
6. Sabine Bernegger, Robert Vidmar, Marko Fonović, Gernot Posselt, Boris Turk, Silja Wessler, "Identification of Desmoglein-2 as a novel target of Helicobacter pylori HtrA in epithelial cells", *Cell communication and signaling*, 2021, **19**, 1, 108.
7. Monika Biasizzo, Mojca Trstenjak-Prebanda, Klemen Dolinar, Sergej Pirkmajer, Janja Završnik, Boris Turk, Nataša Kopitar-Jerala, "Cystatin C deficiency increases LPS-induced sepsis and NLRP3 inflammasome activation in mice", *Cells*, 2021, **10**, 8, 2071.
8. Laura Kist de Ruijter *et al.* (14 authors), "First-in-human study of the biodistribution and pharmacokinetics of $^{89}Zr-CX-072$, a novel immunopet tracer based on an anti-PD-L1 probody", *Clinical cancer research*, 2021, **27**, 19, 5325-5333.
9. Katja Venko, Marjana Novič, Veronika Stoka, Eva Žerovnik, "Prediction of transmembrane regions, cholesterol and ganglioside binding sites in amyloid-forming proteins indicate potential for amyloid pore formation", *Frontiers in molecular neuroscience*, 2021, **14**, 619496.
10. Jure Pražnikar, "Scaling laws of graphs of 3D protein structures", *Journal of bioinformatics and computational biology*, 2021, **19**, 1, 2050050.
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12. Julius Kostan *et al.* (17 authors), "Molecular basis of F-actin regulation and sarcomere assembly via myotilin", *PLoS biology*, 2021, **19**, 4, e3001148.
13. Iñaki Etxeberria *et al.* (24 authors), "Antitumor efficacy and reduced toxicity using an anti-CD137 Probody therapeutic", *Proceedings of the National Academy of Sciences of the United States of America*, 2021, **118**, 26, e2025930118.
14. Marko Fonović, Tamara Leskovar, Iztok Štamfelj, "Določitev spola na podlagi spolno dimorfnih amelogeninskih peptidov v človeški zobni sklenini", *Revija za kriminalistiko in kriminologijo*, 2021, **72**, 2, 117-128.
15. Sebastian Günther *et al.* (102 authors), "X-ray screening identifies active site and allosteric inhibitors of SARS-CoV-2 main protease", *Science*, 2021, **372**, 6542, 642-646.

REVIEW ARTICLE

1. Daniel J. Klionsky *et al.* (2299 authors), "Guidelines for the use and interpretation of assays for monitoring autophagy (4th edition)", *Autophagy*, 2021, **17**, 1, 1-382.
2. Bernarda Majc, Metka Novak, Nataša Kopitar-Jerala, Anahid Jewett, Barbara Breznik, "Immunotherapy of glioblastoma: current strategies and challenges in tumor model development", *Cells*, 2021, **10**, 2, 265.
3. Eva Žerovnik, "Viroporins vs. other pore-forming proteins: what lessons can we take", *Frontiers in chemistry*, 2021, **9**, 626059.
4. Livija Tušar, Aleksandra Usenik, Boris Turk, Dušan Turk, "Mechanisms applied by protein inhibitors to inhibit cysteine proteases", *International journal of molecular sciences*, 2021, **22**, 3, 997.
5. Eva Žerovnik, "On similarities and differences of HIV and SARS Cov-2: open questions relevant for COVID-19 diseas", *Journal biotechnology and biomedicine*, 2021, **4**, 4, 147-158.

SHORT ARTICLE

1. Dušan Turk, Gregor Gunčar, "Thyroxine hormones visualized by the cryo-EM structure of bovine thyroglobulin", *Acta crystallographica. Section D, Structural biology*, 2021, **77**, 1346-1347.

Independent Component Part or a Chapter in a Monograph

1. Olga Vasiljeva, Lisa Sevenich, Thomas Reinheckel, "Analyzing the role of proteases in breast cancer progression and metastasis using primary cells from transgenic oncomice", In: *Metastasis: methods and protocols*, (Methods in molecular biology **2294**), Humana Press, 2021, 275-293.
2. Alexey A. Tsukanov, Olga Vasiljeva, "Nanomaterials interaction with cell membranes: computer simulation studies", In: *Multiscale biomechanics and tribology of inorganic and organic systems*, (Springer tracts in mechanical engineering), Springer, 2021, 189-210.

Patent Application

1. Olga Vasiljeva, Emma Geertruida Elisabeth De Vries, Marjolijn N. Lub-de Hooge, Annelies Jorritsma-Smit, Martin Pool, Danique Giesen, Iris Kok, Linda N. Broer, Mark Stroh, *Positron emission tomography imaging of activatable binding polypeptides and related compositions thereof*, US2020405890 (A1), US Patent Office, 31. 12. 2020.

2. Olga Vasiljeva, Stephen James Moore, Bruce Howng, Susan K. Lyman, Luc Roland Desnoyers, *Methods of qualitatively and/or quantitatively analyzing properties of activatable antibodies and uses thereof*, US2021025877 (A1), US Patent Office, 28. 01. 2021.

Patent

1. Stephen James Moore, Margaret Thy Luu Hyugen, Daniel Robert Hostetter, Olga Vasiljeva, Jason Gary Sagert, Jonathan Alexander Terrett, James William West, *Matrix metalloprotease-cleavable and serine protease-cleavable substrates and methods of use thereof*, US11046759 (B2), US Patent Office, 29. 06. 2021.

Theses and Mentoring

1. Samra Hasanbašić, *Investigating the influence of intrinsic and extrinsic factors on amyloid fibrillation: a study on stefin B model:* doctoral dissertation, Tuzla, 2021 (mentor Eva Žerovnik).
2. Alma Mujkić, *Influence of antioxidants on amyloid fibrillation; in vitro studies on the model of human stefin B and cystatin:* doctoral dissertation, Tuzla, 2021 (mentor Eva Žerovnik).

DEPARTMENT OF MOLECULAR AND BIOMEDICAL SCIENCES B-2

The research programme 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.

Head:
Prof. Igor Križaj

Toxinology

One of our traditional research topics in the field of toxinology is the study of molecular mechanisms of toxic action of secreted phospholipases A_2 ($sPLA_2s$) from animal venoms. In particular we are focused on those endowed with presynaptic neurotoxicity (β-neurotoxins). The knowledge that we are gaining by studying toxic $sPLA_2s$ is helping us to discover the pathophysiological roles of orthologous mammalian $sPLA_2s$, for example, their role in the development of neurodegenerative diseases such as Alzheimer's (AD).

In this year we continued with the characterization of the interaction of ammodytoxin (Atx), a neurotoxic snake venom $sPLA_2$, with its mitochondrial receptor, cytochrome c oxidase (CCOX), to deepen our understanding of motoneuron poisoning by Atx and to shed light on the pathophysiological role of a mammalian group IIA $sPLA_2$ (GIIA), an orthologue of Atx, in this organelle. With this aim, we monitored the intracellular trafficking of derivatives of recombinant Atx, rat GIIA and their enzymatically inactive (D49S) mutants in PC12 cells by transmission electron and fluorescence confocal microscopy. From the results, we concluded that $sPLA_2$ molecules do not require enzymatic activity to enter and traffic within the cell, including entering the mitochondria. A draft article has been prepared to report on this observation. We also continued to investigate the effect of both $sPLA_2s$, Atx and rat GIIA, on mitochondria in PC12 cells. By flow cytometry, we found that GIIA(D49S) slightly reduced mitochondrial potential, whereas GIIA had no significant effect on it. Using ^{125}I-GIIA, we determined the binding affinity of GIIA to a mitochondrial protein with an apparent molecular mass of 20 kDa (R20). Given that GIIA, like Atx, inhibits CCOX activity, we hypothesize that R20 is a subunit of CCOX IV (CCOX-IV). As we were not able to confirm this with the help of anti-CCOX-IV antibodies, we attempted to identify R20 following its isolation from porcine mitochondria. We have synthesized a GIIA-affinity gel, but the conditions for reversible receptor binding to it have not yet been found. A precise description of the action of GIIA on CCOX is crucial for our findings to be used in medicine, both for the early diagnosis of AD as well as for the subsequent treatment of this severe neurodegenerative disease. Namely, it has been shown that GIIA in AD is overexpressed and becomes toxic to mitochondria, which is similar to the effects observed in Atx-poisoned nerve endings.

Animal venoms are a rich source of new substances and molecular tools to improve human and animal health.

It has been demonstrated that certain $sPLA_2s$ specifically bind to nicotinic acetylcholine receptors (nAChRs). Therefore, we have become involved in the research of a specific lung cancer where cancer cells overexpress $\alpha 7$ nAChR, and where natural selective $\alpha 7$ nAChR antagonists are being intensively studied for the development of new target drugs. Using recombinant DNA technology, we have prepared an array of $sPLA_2s$, such as human GV and GX, Atx and rat GIIA, and their enzymatically inactive mutants, GV(H48Q), GX(H48Q), Atx(D49S) and GIIA(D49S). In collaboration with pharmacologists from the University of Leuven, Belgium, we determined the effect of these proteins on $\alpha 7$ and muscle-type nAChRs. Measurements are still ongoing, but the most interesting result was that GV(H48Q) selectively binds only to the $\alpha 7$ form of nAChR, but not to the muscle form. In parallel, we also developed a research model of lung cancer, an A549 lung adenocarcinoma cell line with the overexpression of $\alpha 7$ nAChR, to test the effects of GV(H48Q) and other $\alpha 7$ nAChR antagonists on cell viability, cytotoxicity, proliferation, and apoptosis.

We have prepared two review articles on the topic of $sPLA_2s$. The first, which presents the antiviral activity of both endogenous mammalian and exogenous $sPLA_2s$, i.e., those found in animal toxins, has already been published (J. Pungerčar et al., *Biochimie*, 189 (2021), 40–50). The second one, on the action of $sPLA_2s$ as a consequence of their protein receptor binding, has been accepted for publication (A. Ivanušec et al., *Int. J. Biol. Sci.*, in press). A monograph was also published by the renowned publishing house CRC Press, where I. Križaj participated in the preparation of a chapter on $sPLA_2$ toxins from snake venoms (B. Lomonte and I. Križaj, 2021).

In 2021 we continued with an extensive study of snake-venom proteins that affect the process of blood coagulation – haemostasis. As part of research project J1-2475, we are investigating a unique anticoagulant homologue of serine protease from the venom of the nose-horned viper (*Vipera ammodytes ammodytes*, *Vaa*), VaaSPH-1, in the
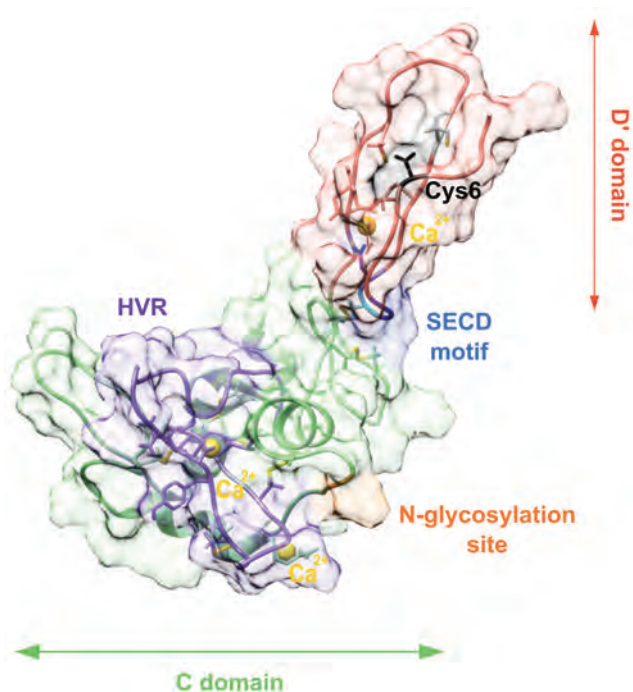
Figure 1: Three-dimensional homologous model of VaaMPIII-3 protein. The structural model of the VaaMPIII-3 protein was prepared by homologous modelling according to the crystal structure of the most similar AaHIV protein from the venom of the crotalid snake Agkistrodon acutus (PDB code: 3HDB). The truncated disintegrin-like part of the molecule (D') is dark orange and the Cys-rich part (C) is green. Cys6, integrin-binding motif (SECD), N-glycosylation site and hypervariable region (HVR) are shown in black, blue, orange and purple. Ca²⁺ ions are represented by yellow beads and disulphide bonds by yellow rods.

direction of developing completely new and safe drugs with anticoagulant action. We searched for the best possible conditions for the expression of VaaSPH-1 in HEK293 suspension cells. In parallel, in collaboration with a US partner from the University of North Carolina (NCATSU), USA, we optimized a three-dimensional *in silico* model of the complex between activated coagulation factor VIII (FVIIIa) and VaaSPH-1, to design low-molecular-mass FIX antagonists for their testing *in vitro*. We have also prepared an invited review article on the topic of serine pseudoproteases (N. Zupanič et al., *FEBS J.*, in press).

After the publication of a detailed description of the VaaSP-VX serine protease, which promotes blood clotting by activating both FV and FX, we began to isolate and characterize a very similar molecule in *Vaa* venom, VaaSP-6. In contrast to VaaSP-VX, we know the entire cDNA sequence of VaaSP-6, which makes it possible to obtain protein in recombinant form. If the recombinant VaaSP-6 exhibits the same unique procoagulant activity as VaaSP-VX, it could replace the dilute Russell's viper venom (dRVV) that is currently used for the clinical determination of lupus anticoagulants (LA test), but is quite unreliable.

We concluded with the extensive genetic, biochemical and physiological characterization of the VaaMPIII-3 protein from the nose-horned viper venom (Figure 1). By analysing its gene structure, we have unequivocally proved that the protein belongs to a special subclass of metalloproteinases from snake venoms, subclass P-IIIe, whose introduction we proposed. We have written an article that is ready to be sent for publication (K. Požek et al., in preparation).

Together with colleagues from the Centre for Clinical Toxicology and Pharmacology, University Medical Centre Ljubljana (UMCL), we investigated an interesting clinical effect in patients envenomed by the nose-horned viper, namely, deep, transient and reversible thrombocytopenia of functional thrombocytopenia, as part of research project J3-2534. In thromboembolic diseases, such as myocardial infarction and ischemic stroke, platelets play a central role. Existing antiplatelet drugs have one common side effect – a reduced number of platelets whose activity is inhibited. This condition poses a high risk of life-threatening bleeding (haemorrhage), especially in interventional cardiology and angiology that use an antithrombotic approach. Our findings may pave the way for the development of a new group of antiplatelet agents that would reduce the risk of dangerous bleeding in such an approach in interventional cardiology and angiology, and increase the effectiveness of vasodilation and clot removal. As shown, reversible thrombocytopenia in patients envenomed by the *Vaa* can be caused by snake proteins similar to type-C lectins (PLTCs, named also snaclecs). Several PLTCs were isolated from *Vaa* venom, and two of them, PLTC3/2 and PLTC1/7, in homogeneous form and in sufficient quantity for detailed characterization. Among other things, we measured their effect on blood clotting and characterized their binding to platelet receptors. High-affinity PLTC3/2 was found to bind to the GPIb receptor (CD42b). The better-labelled PLTC3/2 is ready for an *in vivo* study in mice that will be carried out in cooperation with partners from the Faculty of Veterinary Medicine, University of Ljubljana (VF/UL).

Within the research network, with experts from UMCL, University Hospital and University of Split, University of Zagreb (UZ) and from our group, we analysed samples of patients who were envenomed by the *Vaa* and treated with different antidotes. In the publication, we propose new guidelines for effective immunotherapy in the treatment of *Vaa* envenomation (T. Kurtović et al., *Toxins*, 13 (2021), 279).

Lipid metabolism and signalling

Our research in the field of lipid metabolism and signalling is focused on the role of lipid droplets in cellular stress. These organelles are essential for fat storage and energy production in various tissues, but emerging evidence

Targeting lipid droplets is a promising strategy for the suppression of tumour growth.

has shown that lipid droplets are also crucial for the cellular response to imbalances in energy and redox status. We are particularly interested in the connections between fat storage, inflammatory signalling, autophagy and ferroptosis. This work is of general interest for the wide field of molecular and cell biology, but is particularly applicable to the expanding range of pathophysiological conditions associated with dysregulated lipid metabolism, including cancer, metabolic diseases and neurodegeneration.

In 2021, our experimental work in the scope of the postdoctoral research project Z3-2650 was focused on the study of the roles of lipid droplets in the production of inflammatory lipid mediators (E. Jarc Jovičić et al., *bioRxiv*, doi.org/10.1101/2021.11.25.470010). The results show that lipid droplets not only store polyunsaturated fatty acids (PUFAs) in the form of neutral lipids, but also control their entry into lipid mediator production pathways, thereby implicating lipid droplets in inflammation, immunity and tumourigenesis. We demonstrate that adipose triglyceride lipase (ATGL) promotes the incorporation of lipid droplet-derived PUFAs into phospholipids, which are then targeted by cytosolic PLA_2. This work is important because it identifies a central role of fat storage for the supply of PUFAs into oxygenation pathways. Namely, the control of the availability of PUFAs has been traditionally attributed to PLA_2-dependent membrane phospholipid hydrolysis. Our data suggests that targeting lipid droplet turnover – instead of PLA_2s, which have been proven as unsuitable targets for pharmacological intervention in several clinical trial – could be a valid strategy for reducing inflammation and inflammation-related tumorigenesis.

We continued our work on the research project J7-1818, focused on targeting lipid droplets to reduce cancer-cell resistance to stress. We tackled the question of the cooperation between autophagy and lipid droplets in cancer. Promising preliminary results on ferroptosis (Figure 2) supported the acquisition of another postdoctoral research grant Z3-3211 devoted to the study of the interplay between lipolysis and lipophagy in the modulation of ferroptosis in cancer.

We have contributed to the study of the accumulation of lipid droplets in astrocytes under stress, led by colleagues from the Medical Faculty, University of Ljubljana (MF/UL). We investigated the dynamics of astrocytic lipid-droplet accumulation during nutrient and oxidative stress or noradrenaline exposure, and suggested a neuroprotective role of lipid droplets that accumulated during stress conditions (T. Smolič et al., *Glia*, 69 (2021), 1540–1562).

The scientific community accepted our work on lipid droplets very well, as evident from the rapid increase in the number of citations and lecture invitations, including a presentation at the joint workshop of the EpiLipidNET COST Action and the German Research Council Priority Program on Ferroptosis. We received several awards for our work. The most prestigious, the *FEBS Letters Best Poster Award*, was obtained by our PhD student Špela Koren at the 45th FEBS Congress.

Figure 2: Lipid droplets are anti-oxidant organelles that protect lipids from oxidation. Lipid droplets in MDA-MB-231 breast-cancer cells with compromised redox defences (via glutathione peroxidase 4 (GPX4) inhibition by RSL-3) were stained with the LipiBlue dye (blue) (Dojindo Molecular Technologies) and imaged by live-cell confocal microscopy. The level of lipid peroxidation was estimated by staining cells with the oxidation-sensitive lipophilic probe BODIPY C11 581/591 (Thermo Fischer Scientific). Lipid droplets predominantly contain the reduced form of the dye (red, magenta), suggesting that they provide an antioxidant environment that protects the dye from oxidation (A. Kump et al., in preparation).

High-throughput genetics and functional genomics in yeast *Saccharomyces cerevisiae*

Most traits, including those important for microbial biotechnologically, are polygenic. Therefore, for the past several years our research has been focused on the polygenic traits in the yeast *S. cerevisiae*. In this model organism, we have been studying fundamental aspects of genetics that are also important from a biomedical point of view, as well as developing new, biotechnologically interesting yeast strains.

In the field of the biotechnological application of yeast, we completed and published a study in which we identified and characterized three new causal genes for lipid storage content in common yeast (K. Pačnik et al., BMC Genomics, 22 (2021), 110). We also modified this trait of the yeast as a biotechnologically established organism, which in the future will be able to largely replace the use of other sources of lipids or similar molecules (e.g., oil for energy needs or palm oil for the food industry), in another study published this year (S. Arhar et. al., Microb. Cell Fact., 20 (2021), 147). Here, we made six changes to the yeast genome for the purpose of metabolic engineering. We showed that with only such a relatively small change in the genome a strain capable of accumulating lipids up to 65% of the dry weight could be obtained (Figure 3).

We continued to investigate the molecular mechanisms of the pathogenicity of the SARS-CoV-2 virus. In collaboration with colleagues from the Institute of Microbiology and Immunology (IMI) of the Medical Faculty in Ljubljana, we followed the emergence of virus variants. Specifically, we focused on the variants of the ORF8 protein encoded by viral genomes in Slovenia. Binary protein-protein interactions between variants of the ORF8 viral protein and human proteins were analysed by the two-hybrid yeast system method. We showed that ORF8 specifically interacts with the extracellular domains of three proteins important for the human immune response:

Yeast genetics and genomics for the development of biotechnology and in biomedical research. Integrative genomics for the understanding of covid-19 pathogenesis.

Figure 3: Yeast microscopy under storage lipid accumulation conditions. Left: wild-type strain; right: genetically modified strain. Storage lipids in lipid droplets were stained with the BODIPY 493/503 dye.

TGFB1, ITGB1, and ADAM9. We found that a truncated version of the ORF8 protein encoded by the genomes of a strain of the virus that was prevalent in Slovenia and the world in the middle of 2021 (i.e., the alpha variant) loses the ability to form these interactions. In collaboration with colleagues from IMI and the Clinic for Infectious Diseases of UMCL, we proved that this change does not lead to the loss of pathogenicity of the virus. This has called into question previously published hypotheses that mutations in the ORF8 protein gene lead to the attenuation of SARS-CoV-2 and some other β-coronaviruses.

Evolutionary genomics

The cave salamander or proteus (*Proteus anguinus*) is an animal with exceptional morphological and physiological adaptations to the subterranean environment, with a regenerative ability, a high resistance to prolonged starvation, and a lifespan that may exceed 100 years. To explain the very interesting features of this organism we initiated an analysis of its genome. The genome sequence, estimated to almost 50 Gb, is still unknown. The international Proteus Genome Research Consortium (http://proteusgenome.com) has been established to tackle the challenge of sequencing the proteus genome and its transcriptomes, and funds to initiate the work raised. In the J1-2469 project, led by our colleagues at the Biotechnical faculty UL (BF/UL), we participate with the analysis of genomic and transcriptomic data. Until now, we have obtained initial genomic and transcriptomic data from multiple tissues. DNA sequencing is entering the next phase, the phase of a real-time single molecule sequencing (SMRT), and also sequencing of short DNA transcripts (Figure 4). The genomes of salamanders are exceptionally large (more than 15-fold larger than the human genome) and possess high degrees of repetitive sequences, which makes both sequencing and assembly challenging. Repetitive DNA, made mostly of diverse transposable elements (TEs), is estimated at 90% of the proteus genome size ($\sim$40,5 Gb). Assembly of the genome sequence is thus an extremely difficult task. In 2021 we analysed TEs in the proteus transcriptome and assembled a large collection of TEs (species-specific repetitive library). The ultimate ambition of the proteus project is that we foster, by insight into the proteus genome, medical advancements in the area of aging, tissue regeneration, and therapy of metabolic disorders. The first paper on this subject has been accepted for publication (R. Kostanjšek et al., *Ann. NY Acad. Sci.*, in press).
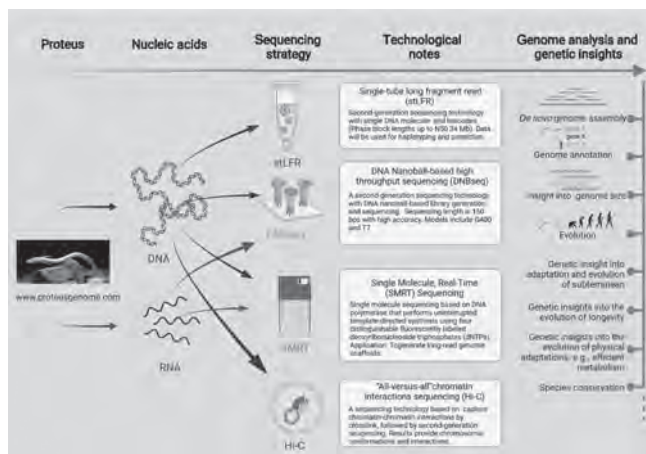
Figure 4: Schematic illustration of the proteus-genome-sequencing plan. Both genomic DNA and RNA are isolated from Proteus anguinus tissue, and sequenced. The proteus-genome structure will provide genetic insights into its evolution and adaptation to the subterranean environment, longevity, metabolism and regeneration, and will aid preservation of this unique animal. The figure is adapted from R. Kostanjšek et al. (Ann. NY Acad. Sci., (2021), in press).

Further, we analysed the origin, diversity and domain architecture of the aerolysin superfamily of protein toxins in basal metazoans (sponges, ctenophores and cnidarians). These toxins that form pores in cell membranes represent one of the most fundamental defence systems of organisms. Proteins of the aerolysin superfamily contain a pore-forming aerolysin domain and a receptor-binding domain (RBD). In contrast to the highly conserved pore-forming domains, RBDs are highly variable, and their structural variations lead to differences in target recognition and, consequently, of the way of action. In numerous genomes and transcriptomes of basal metazoans we discovered unexpectedly large diversity and many novel domain architectures of aerolysin superfamily (D. Kordiš, manuscript in preparation).

Evolutionary, genomic and structure-function analysis of viruses, receptors and satellite DNA.

Other subjects

In 2021 we also participated in different projects that are outside the thematic framework of our department.

We are partners in several research projects funded by the Slovenian Research Agency (ARRS). In the project J1-2482 (the leading institution is BF/UL), we determined the impact of environmentally relevant nano- and microplastics on terrestrial vertebrates by mass spectroscopy, and started preparing an article based on the obtained results. As part of the application project L4-1839 (leading institution: BF/UL), we developed a procedure for the isolation and identification of antimicrobial defensins in chestnut honey for medical use.

We also informally collaborated with several groups at home and abroad. Colleagues from the Ruđer Bošković Institute and UZ were assisted in researching the mechanism of formation and morphogenesis of biomineral nanostructures of the *Archa noae* shell. We performed structural identification of protein components of the shell that are potentially involved in the biomineralization process. The publication is in the process of being reviewed by the journal *Colloid Surf. A: Physicochem. Eng. Asp.* (I. Sondi et al., submitted). In a study led by colleagues from the Faculty of Electrical Engineering UL (FE/ UL), we analysed the protein crown composition of nanoparticles in a proteomic approach to explain their impact on the human immune system. The results were described in an article

under review in the journal *Int. J. Biol. Sci.* (K. Strojan et al., submitted), and another article is in preparation. At the invitation of our colleagues from the same faculty, we also prepared and published a review article on the electroporation of cell membranes (K. Balantič et al., *Acta Chim. Slov.*, 68 (2021), 753–764). We participated in a study of colleagues from VF/UL who were interested in the usefulness of insect proteins for food purposes. Using mass spectroscopy, we searched for potential human allergens in protein preparations. We have already managed to publish this analysis (B. Premrov Bajuk et al., *Animals*, 11 (2021), 1942). To a group from the MF/UL, we came to the aid of research into glioblastoma multiforme (GBM), the most common and deadly form of brain tumour. We collaborated with the confocal microscopic analysis of NB3F18 nanobody as a candidate for selective targeting of glioblastoma cells (Figure 5). A publication on this topic is in the final stages of preparation. We also participated in the preparation of two publications in the field of analysis of trans fatty acids in nutrition (N. Zupanič et al., *Nutrients*, 13 (2021), 207 and A. Kušar et al., *Public Health Nutr.*, 24 (2021), 12–21).

Following the outbreak of the covid-19 pandemic in 2020, we began a two-year expanded programme activity aimed at researching various aspects of the functioning and evolution of SARS-CoV-2. We are completing the planned research and preparing publications.
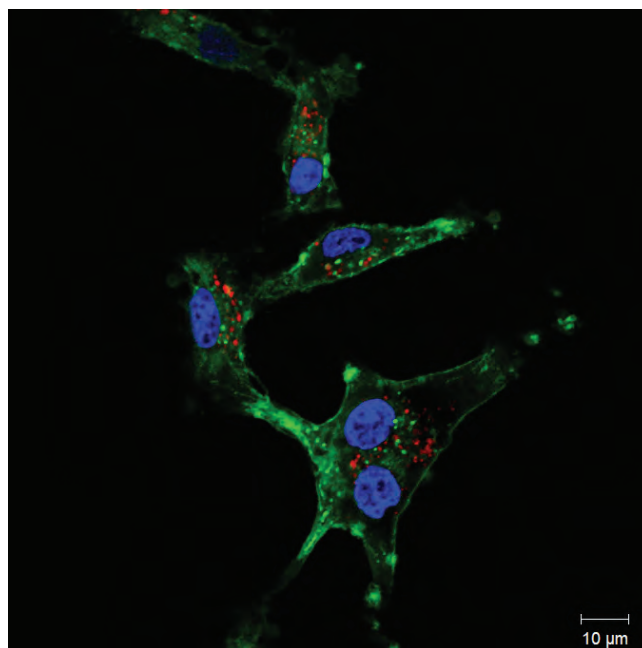
Figure 5: Confocal microscopy of glioblastoma cells. The NB3F18 nanobody (red) recognizes the target antigen on U87MG glioblastoma cells. The membranes are coloured green (BioTracker Green) and nuclei blue (DAPI).

Some outstanding publications in the past year

1. Lomonte, B. and Križaj, I. (2021): Snake venom phospholipase A_2 toxins. In: Handbook of Venoms and Toxins of Reptiles, 2nd Edn. (Stephen P. Mackessy; Ed.). ISBN 9780367149741. CRC Press; Taylor & Francis Group, Boca Raton, Florida, USA; pp. 389–411

2. Kurtović, T., Karabuva, S., Grenc, D., Dobaja Borak, M, Križaj, I., Lukšić, B., Halassy, B. and Brvar, M.: Intravenous *Vipera berus* Fab fragments and intramuscular *Vipera ammodytes* F(ab')$_2$ fragments in *Vipera ammodytes* envenomed patients. Toxins, 13 (2021), 279

3. Pungerčar, J., Bihl, F., Lambeau, G. and Križaj, I.: What do secreted phospholipases A_2 have to offer in combat against different viruses up to SARS-CoV-2? Biochimie, 189 (2021), 40–50

4. Pačnik, K., Ogrizović, O., Diepold, M., Eisenberg, T., Žganjar, M., Žun, G., Kužnik, K., Gostinčar, C., Curk, T., Petrovič, U. and Natter, K.: Identification of novel genes involved in neutral lipid storage by quantitative trait loci analysis of *Saccharomyces cerevisiae*. BMC Genomics, (22) 2021, 110

5. Arhar, S., Gogg-Fassolter, G., Ogrizović, M., Pačnik, K., Schwaiger, K., Žganjar, M., Petrovič, U. and Natter, K.: Engineering of *Saccharomyces cerevisiae* for the accumulation of high amounts of triacylglycerol. Microb. Cell Fact., (20) 2021, 147

Awards and Appointments

1. Sabina Drofenik: Krka recognition 2021, Novo mesto, Krka, pharmaceutical company. Research project: Description of the mechanism and interdependence of the action of two nose-horned viper venom proteins, secretory phospholipase A_2 and chymotrypsin inhibitor (co-mentor prof. Igor Križaj).

2. Adrijan Ivanušec, Jernej Šribar, Peter Veranič, Maja Zorovič, Marko Živin and Igor Križaj: Best Poster Award: 8th Oxford Venoms and Toxins Meeting (virtual), Work title: Mammalian secreted phospholipase A_2 group IIA binds to the same mitochondrial receptor as its β-neurotoxic orthologue from snake venom.

3. Kity Požek, Adrijana Leonardi, Milan Kojić and Igor Križaj: Best Poster Award: 8th Oxford Venoms and Toxins Meeting (virtual), Work title: Production and characterization of recombinant VaaMPIII-3, a disintegrin like/cysteine rich protein from *Vipera a. ammodytes* venom.

4. Kity Požek: Best essay competition: Hamish Ogston Foundation, London, United Kingdom, Work title: The impact of the Covid-19 pandemic on snakebite research and treatment.

Organization of conferences, congresses and meetings

1. Igor Križaj, Member of the International Scientific Committee, 45th FEBS Congress (virtual), 3.-8. 7. 2021, Ljubljana.

Jožef Stefan Institute

INTERNATIONAL PROJECTS

1. COST CA19144 - EUVEN; European Venom Network
   Prof. Igor Križaj
   COST Association AISBL
2. COST CA19105 - LipidNET- Pan-European Network in Lipidomics and Epilipidomics
   Prof. Toni Petan
   COST Association AISBL
3. Do Endogenous Secreted Phospholipases A$_2$ Modulate Nicotinic Acetylcholine Receptor Functions?
   Prof. Igor Križaj
   Slovenian Research Agency

RESEARCH PROGRAMME

1. Toxins and biomembranes
   Prof. Igor Križaj

R&D GRANTS AND CONTRACTS

1. Neurotoxicity or neuroprotection of nanomaterials: the rele of biocorona
   Prof. Igor Križaj
2. Protein complexes from the fungal genus Pleurotus, new biopesicides for controlling Colorado potato beetle and western corn rootworm
   Prof. Igor Križaj
3. Exploitation of a virus-borne small protein to combat antibiotic resistance in Staphylococcus aureus
   Prof. Igor Križaj

4. Genomic and transcriptomic insights into the exceptional biology of proteus (Proteus anguinus)
   Prof. Dušan Kordiš
5. Impact of environmentally relevant nano- and micro-plastics on soil invertebrates
   Prof. Igor Križaj
6. Inflammatory process in interstitial cystitis and evaluation of the influence of cannabinoid receptor agonists in urinary bladder - from cells to patients
   Prof. Igor Križaj
7. „Reversibility of transient thrombocytopenia induced by a snake venom component offers asafe antithrombotic prevention in interventional angiology and cardiology"
   Prof. Igor Križaj
8. Neuropsychological dysfunctions caused by low level exposure to selected environmental pollutants in susceptible population – NEURODYS
   Prof. Igor Križaj
9. Targeting lipid droplets to reduce cancer cell resistance to stress
   Prof. Toni Petan
10. Development of an innovative drug to treat venous thromboembolism based on a unique viper venom anticoagulant
    Prof. Igor Križaj
11. Magnetically-controllable nanocarriers mimicking endogenous lipid particles for improved drug/nanoparticle delivery
    Prof. Igor Križaj
12. Development of medical chestnut honey quality control and technology
    Prof. Igor Križaj
13. Hierarchical DNA assembly for advanced applications in biopharmaceuticals production and cell therapy
    Prof. Uroš Petrovič
14. OLEOFERM - Sustainable oleochemicals biopreoduction from carboxylates via oleaginous fermentation
    Prof. Uroš Petrovič
    Ministry of Education, Science and Sport

STAFF

Researchers
1. Prof. Dušan Kordiš
2. **Prof. Igor Križaj**, Head
3. Asst. Prof. Adrijana Leonardi
4. Prof. Toni Petan
5. Prof. Uroš Petrovič*
6. Prof. Jože Pungerčar
7. Dr. Jernej Šribar
Postdoctoral associates
8. Dr. Mauro Danielli
9. Dr. Eva Jarc Jovičić
10. *Dr. Mojca Ogrizović, left 01.12.21*
11. Dr. Nina Zupanič
Postgraduates
12. Tadeja Bele, M. Sc.

13. Adrijan Ivanušec, B. Sc.
14. Špela Koren, B. Sc.
15. Ana Kump, B. Sc.
16. Mia Žganjar, B. Sc.
17. Gašper Žun, B. Sc.
Technical officer
18. Kity Požek, B. Sc.
Technical and administrative staff
19. Igor Koprivec
20. Maja Šimaga, M. Sc.

Note:

* part-time JSI member

BIBLIOGRAPHY

ORIGINAL ARTICLE

1. Katja Balantič, Damijan Miklavčič, Igor Križaj, Peter Kramar, "The good and the bad of cell membrane electroporation", *Acta chimica slovenica*, 2021, **68**, 4, 753-764.
2. Blanka Premrov Bajuk, Petra Zrimšek, Tina Kotnik, Adrijana Leonardi, Igor Križaj, Breda Jakovac-Strajn, "Insect protein-based diet as potential risk of allergy in dogs", *Animals*, 2021, **11**, 7, 1942.
3. Julieta Marrone, Mauro Danielli, César I. Gaspari, Alejo M. Capiglioni, Raúl Marinelli, "Aquaporin gene transfer for hepatocellular cholestasis", *Biochimie*, 2021, **188**, 12-15.
4. Mauro Danielli, Alejo M. Capiglioni, Julieta Marrone, Raúl Marinelli, "Further evidence for the involvement of mitochondrial aquaporin-8 in hepatocyte lipid synthesis", *Biochimie*, 2021, **188**, 16-19.
5. Klavdija Pačnik *et al.* (11 authors), "Identification of novel genes involved inneutral lipid storage by quantitative traitloci analysis of Saccharomyces cerevisiae", *BMC genomics*, 2021, **22**, 110.
6. Tina Smolič *et al.* (12 authors), "Astrocytes in stress accumulate lipid droplets", *Glia*, 2021, **69**, 6, 1540-1562.
7. Simon Arhar, Gabriela Gogg-Fassolter, Mojca Brložnik, Klavdija Pačnik, Katharina Schwaiger, Mia Žganjar, Uroš Petrovič, Klaus Natter, "Engineering of *Saccharomyces cerevisiae* for the accumulation of high amounts of triacylglycerol", *Microbial cell factories*, 2021, 20, 1, 147.
8. Nina Zupanič *et al.* (12 authors), "Dietary intake of trans fatty acids in the Slovenian population", *Nutrients*, 2021, **13**, 1, 207.
9. Anita Kušar *et al.* (16 authors), "Assessment of trans-fatty acid content in a sample of foods from the Slovenian food supply using a sales-weighting approach", *Public health nutrition*, 2021, **24**, 1, 12-21.
10. Tihana Kurtović, Svjetlana Karabuva, Damjan Grenc, Mojca Dobaja, Igor Križaj, Boris Lukšić, Beata Halassy, Miran Brvar, "Intravenous Vipera berus Venom-specific Fab fragments and intramuscular Vipera ammodytes venom-specific F(ab')2 fragments in Vipera ammodytes-Envenomed patients", *Toxins*, 2021, **13**, 4, 279.

Review Article

1. Jože Pungerčar, Franck Bihl, Gérard Lambeau, Igor Križaj, "What do secreted phospholipases A_2 have to offer in combat against different viruses up to SARS-CoV-2?", *Biochimie*, 2021, **189**, 40-50.
2. Anita Kušar, Katja Žmitek, Liisa Lähteenmäki, Monique Raats, Igor Pravst, "Comparison of requirements for using health claims on foods in the European Union, the USA, Canada, and Australia/New Zealand", *Comprehensive reviews in food science and food safety*, 2021, **20**, 2, 1307-1332.

Published Conference Contribution

1. Tadej Markuš, Mladen Soldat, Gregor Kosec, Uroš Petrovič, Martin Kavšček, "Development of platform technology for biotechnological production of carotenoids", In: *Mikrobiološke ideje na prepihu*, zbornik prispevkov, Biotehniška fakulteta, Oddelek za živilstvo, 2021, 101-112.

Independent Component Part or a Chapter in a Monograph

1. Bruno Lomonte, Igor Križaj, "Snake venom phospholipase A_2 toxins", In: *Handbook of venoms and toxins of reptiles*, 2nd ed., CRC Press, 2021, 385-407.

Encyclopaedia, Dictionary, Lexicon, Manual, Atlas, Map

1. Jernej Šribar, Jerica Sabotič, *Navodilo za delo z ultracentrifugo Beckman Coulter Optima XPN-90: poslovna tajnost*, Institut Jožef Stefan, 2021.

Theses and Mentoring

1. Sabina Ott Rutar, *Phylogenomic analysis of RNA viruses in invertebrates:* doctoral dissertation, Ljubljana, 2021 (mentor Dušan Kordiš).

DEPARTMENT OF BIOTECHNOLOGY
B-3

At the Department of Biotechnology we investigate biological molecules of animal, plant microbiological and fungal origin using modern biotechnological methods. We would like to apply them for diagnostic and therapeutic purposes in human and veterinary medicine, for plant protection, the preparation of high-quality and safe food and for the protection of the environment, contributing to an improvement in people's health and the environment in which we live. Our research work is focused on processes of cancer progression and immune response, neurodegenerative processes, the biology of fungi and in the search for new biotechnological approaches and products.

Head:
Prof. Boris Rogelj

Regulation of anti-tumour immune response

We continued our studies of the role of cysteine peptidases and their inhibitors in the regulation of anti-tumor immune response. We focused our work on the endogenous inhibitor cystatin F. It is an important modulator of the cell cytotoxicity of natural killer cells and cytotoxic T cells. Its role in the regulation of anti-tumor immune response we evaluated in patients with glioblastoma. In a tumour micro-environment various cells express and secrete inactive dimeric cystatin F, which can be internalized to cytotoxic cells, activated within endo/lysosomal vesicles, impairing cytotoxic action against tumour cells and cancer stem cells. Consequently, patients with higher levels of cystatin F experience worse disease outcomes than those with low levels. In addition, in natural killer cells and cytotoxic lymphocytes, we also demonstrated the regulatory role of cystatin F in helper T cells (CD4+) and found the association between its expression and the clonal expansion of CD4+ cells. Cystatin F is, therefore, an important mediator employed by tumour cells to impair the killing efficiency of cytotoxic cells. It represents a possible target for cancer immunotherapy. For this purpose, we investigated the action of inhibitors of the peptidase, which activates an intact dimeric cystatin F into an active one as well as various regulators of glycosylation, which can prevent the access of cystatin F to its targets within endo/lysosomal pathway.

Molecular neurodegeneration

With an aging population and the lack of a useful therapy, neurodegenerative diseases are increasing and becoming one of the leading causes of death worldwide. In this field our main focus is on selected genes and their protein products (TDP-43, FUS, C9orf72, SFPQ, MATR3, etc.) associated with amyotrophic lateral sclerosis (ALS), frontotemporal dementia (FTD) and Alzheimer's disease (AD). The majority of them are in some way associated with RNA biogenesis, processing, transport and turnover. We study their nuclear transport, cellular stress response and macromolecular interactions leading to mislocalization and aggregation.

Because the protein interactors of FUS causative of its cytoplasmic toxicity are still unknown, we used BioID2 proximity labelling to identify the interactomes of FUS and FUSdNLS (without NLS) proteins overexpressed in the HEK293T cells. Our bio-informatic analyses identified interactors involved in RNA processing and degradation, protein translation and pro-survival (FGF) or inhibitory (TGF) signalling pathways. In-vitro analyses showed that FUS interacts with NUDT21 (Nudix hydrolase 21, cleavage factor subunit) and decreases its nuclear expression, whereas the interaction with NUDT21 is abolished by FUSdNLS, possibly having downstream effects on 3'RNA cleavage and polyadenylation, leading to the toxic disruption of neuronal homeostasis. We generated the stable cell lines Flp-In HEK293 and Flp-In SH-SY5Y, expressing KO2-wtTDP-43-HA, KO2-dNLS-TDP-43-HA or KO2-only. We have also obtained mouse-brain samples with a TDP-43 ALS pathology that will be used to detect interactors identified in BioID-TDP-43 experiments. To determine changes in the interactome of TDP-43 during stress-granules formulation and dissolution, we generated four stable cell lines expressing APEX-myc-wtTDP-43, APEX-myc-dNLS-TDP-43, APEX-
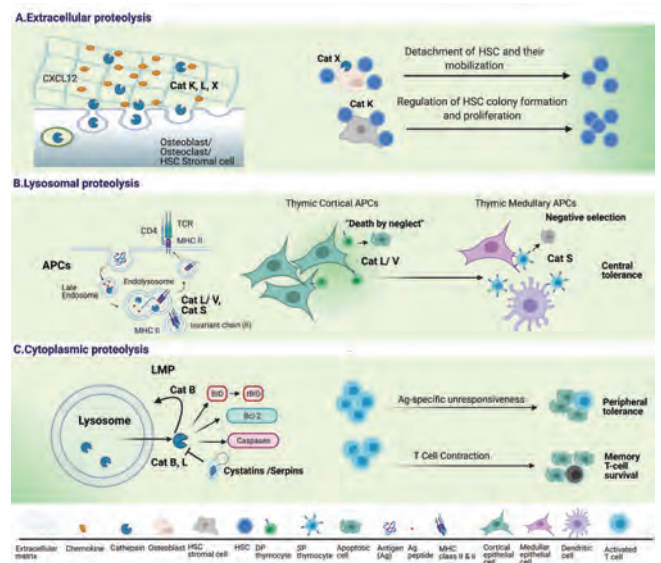
Figure 1: Regulation of T lymphocyte survival by cysteine cathepsins

Cystatin F in a tumour micro-environment impairs the cytotoxic function of T cells and natural killer cells.
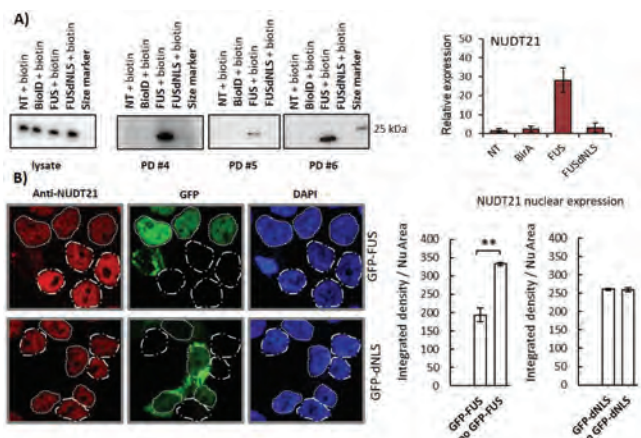
Figure 2: Identifying NUDT21 as a FUS interactor. A) Western blots of BioID2-labelled interactors isolates, showing NUDT21 interaction with FUS as confirmed by NUDT21 25kDa band (left) and signal quantified (right) B) Cells transfected with GFP-FUS and GFP-FUSdNLS showing decrease in nuclear NUDT21 expression as compared to non-transfected cells (left) and signal quantified (right).

myc-CT-TDP-43 and APEX-myc. In addition, we determined the timecourse of the stress granules' dissolution.

In our study published in *Brain*, we focused on poly-dipeptide repeats resulting from the translation of mutant repeat expansions in the C9orf72 gene that accumulate in cells as aggregates and cause cell death in neurodegenerative diseases. We also used BioID2 proximity labelling to identify the interactomes of all five dipeptides repeat proteins (polyGA, polyGR, polyPR, polyPA and polyGP), each consisting of 125 repeats. We identified their interaction partners and, using autopsy brain tissue from patients with C9orf72 expansion complemented with cell culture analysis, examined the interactions between polyGA and valosin-containing protein (VCP). Our unique functional analysis of this interaction revealed the sequestration of VCP with polyGA aggregates, which alters the concentration of soluble VCP protein and inhibits autophagy. We also determined the effect of C4G2 repeat on phenylalanine-tRNA synthetase. We have shown that there is a lower level of charged tRNAphe in the presence of repeats and that C4G2 inhibits the function of FARS protein in in-vitro studies. Additionally, we have shown that the interaction between C4G2 and FARS reduces the expression level of phenylalanine-rich proteins in lymphoblasts with C9orf72 mutation compared to controls. We have developed a Click-chemistry protocol with mutated FARSA protein, which enables the incorporation of azido-phenylalanine into proteins, for observing the changes in the global effect of C4G2 repeats on protein synthesis.

Prader Willi syndrome and RNA biology

In 2021 we also optimised the protocol for COMRADES, which is used to obtain SNORD116 interactors. We prepared a PARIS and COMRADES library of interactors from the SHSY5Y cell line. Since the obtained library did not show the expected results during the validation steps we focused on optimising the protocol even further in order to obtain better libraries for sequencing.

Probiotics

We continued our work on the targeting of colorectal cancer cells by recombinant *Lactococcus lactis,* a safe, food-grade bacterium from the group of lactic acid bacteria. The binding of engineered bacteria to cancer cells would enable the selective delivery of biopharmaceuticals by the bacteria and avoid side effects. Targeting was achieved by displaying on the bacterial surface two small protein binders of tumour-specific antigens, namely EpCAM and HER2, that are present on cancer cells. The functionality of the bacteria was further increased by the co-expression of an infrared fluorescent protein that enabled the imaging of bacteria. We confirmed the binding of engineered *L. lactis* to soluble forms of EpCAM and HER2 using flow cytometry and western blot, and demonstrated the proof-of-principle of targeting on human cell lines HEK293, HT-29 and Caco-2. The engineered *L. lactis* was selective and no binding was observed to HEK293 cells without tumour antigens. Apart from cell targeting in static conditions, we also demonstrated the targeting ability of engineered *L. lactis* in the conditions of constant flow of bacterial suspension over the HEK293 cells in an advanced fluidic system, thereby emulating the conditions in the gastrointestinal tract.

We engineered *Lactococcus lactis* bacteria that display tumour-antigen binders and selectively attach to cancer cells.
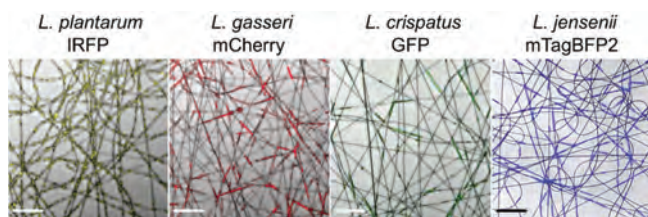
Figure 3: Representative microscopy images of nanofibers containing different species of lactobacilli (Lactobacillus crispatus ATCC 33820, Lactobacillus gasseri ATCC 33323 in Lactobacillus jensenii ATCC 25258) expressing fluorescent proteins IRFP, mCherry, GFP and mTagBFP2 with different spectral properties. Bar: 20 µm.

Fungi contain substances that inhibit the formation of bacterial biofilms.

The above research revealed the need for a simple and modular construction of multigene plasmids and the controlled simultaneous expression of multiple proteins in *L. lactis*. For that purpose, we have introduced in *L. lactis* a modified BglBrick system, originally developed in *Escherichia coli* that the enables straightforward assembly of multiple gene cassettes. Six different expression cassettes, encoding model proteins, were assembled in different order as parts of a modified BglBrick system in a novel plasmid pNBBX. We expressed model proteins either alone or concomitantly, and demonstrated the first controlled expression of three model proteins in *L. lactis*, with considerable biotechnological potential in the synthetic biology of lactic acid bacteria.

Lactic acid bacteria, particularly lactobacilli, are part of healthy vaginal microbiota and could be used to balance vaginal dysbiosis. We have incorporated model vaginal lactobacilli *Lactobacillus crispatus* ATCC 33820, *Lactobacillus gasseri* ATCC 33323, and *Lactobacillus jensenii* ATCC 25258 in poly(ethylene oxide) nanofibers, a potential novel vaginal delivery system for probiotics. To facilitate the study of their distribution and mechanism of action, we have engineered them to express fluorescent proteins with different spectral properties. This enabled quantification and discrimination between lactobacilli cells in nanofibers by using fluorescent microscopy, as well as in suspension after nanofiber dissolution, by measuring the fluorescence. The approach will allow the tracking of probiotics in future delivery studies.

Glycobiology

In the field of glycobiology, we continued to explore the molecular mechanisms of bacterial biofilm development, using the pathogenic bacterium Listeria as a model. Based on an analysis of the results of whole genome random mutagenesis studies and a review of the literature, we reviewed the current understanding of the role of the individual structures that make up the cell wall in the development of Listeria biofilms on abiotic surfaces. Understanding the relationships between surface structures involved in biofilm formation and virulence factors is very important because biofilms allow bacteria to survive long term in different environments. Understanding the role of these structures will help to develop new strategies to combat microorganisms that pose the greatest threat to human and animal health. In addition, in collaboration with Prof. Paola Cescutti from the University of Trieste and others, we determined the structure of teichoic acid from the cell wall of Listeria innocua ŽM39. It turned out to be a new type of structure of teichoic acid in Listeria, and similar to the structure characteristic of serovar 6a. Sequencing and annotation of the genome of this strain also allowed the identification of predicted genes for the biosynthesis of teichoic acid.

Figure 4: Listeria innocua ŽM39 cell-wall teichoic acid.

In the field of fungal bioactive proteins we continued research on antimicrobial activities in 2021. It is important to distinguish between antimicrobial (affecting growth) and antibiofilm (affecting biofilm) activities because antimicrobial drugs that affect bacterial growth cause selection pressure that leads to the rapid development of antimicrobial resistance. Therefore, the further development of alternatives to antibiotics focuses, among other things, on agents that do not affect bacterial growth and act on the biofilm to prevent the persistence of infection in a given environment. In collaboration with the Biotechnical Faculty of the University of Ljubljana, we developed a new method to distinguish between antimicrobial activity and antibiofilm activity on a model of the pathogenic bacterium Salmonella. The approach of using the growth curve for the simultaneous analysis of antimicrobial and antibiofilm activity is a methodological novelty, which is why we filed a patent application for it. This simple approach was named Simba and was awarded 3rd place in the University of Ljubljana Rector's Award for the best innovation in 2021. The Simba approach was also tested by studying extracts from 38 wild and 4 cultivated mushroom species. It was found that the toothed jelly fungus (Pseudohydnum gelatinosum) had antimicrobial activity, the oyster mushroom (Pleurotus ostreatus) had antibiofilm activity, and the trooping funnel mushroom (Infundibulicybe geotropa) had both activities.

COVID-19 associated research

We continued our research on the role of cysteine peptidases in the replication and infection of the SARS-CoV-2 virus. For compounds from our peptidase inhibitor library we found the most promising antiviral effect for cathepsin B inhibitors, including antibiotic nitroxoline. The virus uptake to host cells explores two main mechanisms, membrane fusion and endocytosis. They differ regarding peptidases involved in the cleavage of the S protein, in endocytosis the crucial peptidases are cathepsins B and L. It is now known that different variants of SARS-CoV-2 virus prefer one or another mechanism, Omicron, for example, utilizes an endocytic pathway for cell entry. In this case the inhibitors of cathepsins B and L represent a first line in antiviral therapy. At the transition of the Covid-19 from pandemic to endemic phase, besides vaccines antiviral drugs will be the most important to control the disease. For the application of cysteine peptidase inhibitors in antiviral therapy, a PCT patent application was filed.

The results of the research work at the Department of Biotechnology in 2021 were published in 20 scientific papers in journals with an impact factor. We also published eight reviews. We received two new research grants from the Slovenian Research Agency. Urša Čerček received Krka and Prešern awards, while dr. Jerica Sabotič and dr. Ana Mitrovič were mentors for two Krka awards. Members of the department were very also active in pedagogical work as lecturers and mentors to students preparing diploma and doctoral theses at universities in Slovenia and abroad. In 2021 two doctoral theses were completed at the department.

Some outstanding publications in the past year

1. Rheenen, Wouter Van, Van Der Spek, Rick A. A., Bakker, Mark K., Van Vugt, Joke J. F. A., Hop, Paul J., ..., Rogelj, Boris, Koritnik, Blaž, Zidar, Janez, Ravnik-Glavač, Metka, Glavač, Damjan, et al. Common and rare variant association analyses in amyotrophic lateral sclerosis identify 15 risk loci with distinct genetic architectures and neuron-specific biology. *Nature genetics*, ISSN 1061-4036, Dec. 2021, vol. 53, no. 12, str. 1636-1648, ilustr. https://www.nature.com/articles/s41588-021-00973-1, doi: 10.1038/s41588-021-00973-1. [COBISS.SI-ID 88131075] IF 38,3.

2. Pasha, Terouz, Zatorska, Anna, Sharipov, Daulet, Rogelj, Boris, Hortobagyi, Tibor, Hirth, Frank. Karyopherin abnormalities in neurodegenerative proteinopathies. *Brain : journal of neurology*, ISSN 0006-8950, 2021, vol. 144, no. 10, str. 2915%2932, doi: 10.1093/brain/awab201. [COBISS.SI-ID 87473667] IF 13,5.

3. Perišić, Milica, Pečar Fonović, Urša, Jakoš, Tanja, Kos, Janko. The role of cysteine peptidases in hematopoietic stem cell differentiation and modulation of immune system function. *Frontiers in immunology*, ISSN 1664-3224, 2021, vol. 12, str. 680279-1–680279-19, doi: 10.3389/fimmu.2021.680279. [COBISS.SI-ID 71732995] IF 7,6.

4. Senjor, Emanuela, Perišić, Milica, Breznik, Barbara, Mitrović, Ana, Mlakar, Jernej, Rotter, Ana, Porčnik, Andrej, Lah Turnšek, Tamara, Kos, Janko. Cystatin F acts as a mediator of immune suppression in glioblastoma. *Cellular oncology*, ISSN 2211-3436, 2021, vol. 44, no. 5, str.1051-1063, doi: 10.1007/s13402-021-00618-9. [COBISS.SI-ID 69253379] IF 6,7.

5. Stojanov, Spase, Plavec, Tina Vida, Kristl, Julijana, Zupančič, Špela, Berlec, Aleš. Engineering of vaginal lactobacilli to express fluorescent proteins enables the analysis of their mixture in nanofibers. *International journal of molecular sciences*. 2021, vol. 22, no. 24, str. 13631-1-13631-18, ilustr. ISSN 1422-0067. DOI: 10.3390/ijms222413631. [COBISS.SI-ID 90159363] IF 5,9.

6. Plavec, Tina Vida, Mitrović, Ana, Perišić, Milica, Štrukelj, Borut, Kos, Janko, Berlec, Aleš. Targeting of fluorescent Lactococcus lactis to colorectal cancer cells through surface display of tumour-antigen binding proteins. *Microbial biotechnology*. [Online ed.]. 2021, vol. 14, iss. 5, str. 2227-2240, graf. prikazi. ISSN 1751-7915. DOI: 10.1111/1751-7915.13907. [COBISS.SI-ID 73046275] IF 5,8.

7. Janež, Nikolaja, Škrlj, Blaž, Sterniša, Meta, Klančnik, Anja, Sabotič, Jerica. The role of the Listeria monocytogenes surfactome in biofilm formation. *Microbial biotechnology*, ISSN 1751-7915. [Online ed.], Jul. 2021, vol. 14, iss. 4, str. 1269-1281, ilustr. https://sfamjournals.onlinelibrary.wiley.com/doi/10.1111/1751-7915.13847, doi: 10.1111/1751-7915.13847. [COBISS.SI-ID 67146499] IF 5,8.

Awards and Appointments

1. Jerica Sabotič: 3rd place in the University of Ljubljana Rector's Award for the best innovation in 2021, Ljubljana, University of Ljubljana Rector prof. dr Gregor Majdič, SIMBA – Simultaneous detection of antimicrobial and antibiofilm activities.

2. Emanuela Senjor: Dean's Award, Ljubljana, Slovenia, University of Ljubljana, Faculty of Pharmacy, for the paper Cystatin F acts as a mediator of immune suppression in glioblastoma published in Cellular oncology.

3. Abida Zahirović: Krka Prize with special recognition for PhD thesis, Novo mesto, Krka, Identification and characterization of major bee venom allergen Api m 1 mimotopes for development of specific immunotherapy.

Organization of conferences, congresses and meetings

1. Aleš Berlec: 45th FEBS Congress, Ljubljana (virtual), 3. 7. – 8. 7. 2021
2. Ana Mitrović, Minisymposium, Data from the field on biomolecular interactions (virtual), 25. 11. 2021
3. Jerica Sabotič: 20th FEBS Young Scientist's Forum, Lovran, Croatia (virtual), 15. 6. –18. 6. 2021

INTERNATIONAL PROJECTS

1. COST CA18238; Ocean4Biotech - European Transdisciplinary Networking Platform for Marine Biotechnology
    Dr. Jerica Sabotič
    Cost Association Aisbl

2. COST CA19123 - PHOENIX; Protection, Resilience, Rehabilitation of Damaged Environment
    Prof. Aleš Berlec
    Cost Association Aisbl

3. Neuropathological Evaluation of the In Vivo Interactomes of TDP-43, FUS and MATR3 in Human ALS and FTD
    Prof. Boris Rogelj
    Slovenian Research Agency

4. Crosstalk of Proteinopathy and Inflammation in Amyotrophic Lateral Sclerosis
    Prof. Boris Rogelj
    Slovenian Research Agency

RESEARCH PROGRAMME

1. Pharmaceutical Biotechnology: Knowledge for Health
   Prof. Janko Kos

R & D GRANTS AND CONTRACTS

1. Pathogenic role of paraspeckle-like nuclear bodies in neurodegenerative diseases ALS and FTD
   Prof. Boris Rogelj
2. Inhibition of cathepsin X activity as a novel strategy for the treatment of Parkinson's disease
   Prof. Janko Kos
3. Targeting Campylobacter adhesion in the fight against antimicrobial resistance
   Dr. Jerica Sabotič
4. Bactericidal nanoblades: a proof-of-concept approach for bimodal chemo-mechanicaleradication of persistent biofilms
   Dr. Jerica Sabotič
5. Cathepsins B and X in breast cancer stem cells – molecular targets and relevance for antitumor therapy
   Dr. Ana Mitrović
6. Intra-biofilm dynamics of Campylobacter with other bacteria: effects on biofilm formation and composition with a view to the design of innovative control strategies
   Dr. Jerica Sabotič
7. Recombinant probiotics as bio-alternative antimicrobial approach against Clostridioides difficile
   Prof. Aleš Berlec
8. Molecular mechanisms of specificity in regulation of secretion and action of muscle-derived cytokines
   Prof. Boris Rogelj
9. Targeting, imaging and treating of colorectal cancer with safe theranostic bacteria
   Prof. Aleš Berlec
10. Phase transitions in systems of nucleotide repeat expansions associated with neurodegenerative diseases
    Prof. Boris Rogelj
11. New antimicrobial strategies in prevention of biofilm formation by using lectins that inhibit bacterial adhesion
    Dr. Jerica Sabotič
12. Improvement of immunotherapeutic potential of NK cells through modulation of cystatin F
    Prof. Janko Kos
13. Nuclear transport defects in frontotemporal dementia
    Prof. Boris Rogelj
14. Cystatin f as a mediator of immunosuppression in glioblastoma microenvironment
    Dr. Milica Perišić Nanut
15. FunContrAPest: Novel Fungal Proteins as Biopesticides for Control of Challenging Invasive Alien Agricultural Pests
    Dr. Jerica Sabotič
16. Small protein blockers of IL-23/IL-17 axis as intestinal inflammation inhibitors secreted by probiotic bacteria
    Prof. Aleš Berlec
17. Targeting protein phase separation and aggregation in neurodegenerative TDP-43 proteinopathies
    Prof. Boris Rogelj
18. Innovative ECO plasma seed treatment (for sowing and for human and animal diet/nutrition)
    Prof. Boris Rogelj
    Ministry of Education, Science and Sport
19. Cell4Chem: Engineering microbial communities for the conversion of lignocellulose into medium-chain carboxylates
    Prof. Aleš Berlec
    Ministry of Education, Science and Sport

STAFF

Researchers
1. Prof. Aleš Berlec
2. Prof. Janko Kos*
3. Asst. Prof. Helena Motaln
4. Dr. Milica Perišić Nanut
5. **Prof. Boris Rogelj, Head**
6. Dr. Jerica Sabotič
7. Prof. Borut Štrukelj*
Postdoctoral associates
8. Dr. Nikolaja Janež
9. *Dr. Mirjana Malnar, left 01.09.21*
10. Dr. Ana Mitrović
11. *Dr. Eva Ogorevc, left 01.05.21*
12. Dr. Tina Vida Plavec
13. *Dr. Mateja Prunk, left 01.07.21*
14. Dr. Abida Zahirović
Postgraduates
15. Urša Čerček, B. Sc.
16. Emanuela Senjor, B. Sc.
17. Petra Štravs, B. Sc.
Technical officers
18. Tadeja Tumpej, B. Sc.
19. Tanja Zupan, B. Sc.
Technical and administrative staff
20. Maja Šimaga, M. Sc.

Note:

* part-time JSI member

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ORIGINAL ARTICLE

1. Tomaž Marš *et al.* (11 authors), "Innervation and electrical pulse stimulation - in vitro effects on human skeletal muscle cells", *Applied physiology, nutrition and metabolism*, 2021, **46**, 4, 299-308.
2. Terouz Pasha, Anna Zatorska, Daulet Sharipov, Boris Rogelj, Tibor Hortoba´gyi, Frank Hirth, "Karyopherin abnormalities in neurodegenerative proteinopathies", *Brain: journal of neurology*, 2021, **144**, 10, 2915–2932.
3. Anja Pišlar, Janko Kos, "γ-enolase enhances Trk endosomal trafficking and promotes neurite outgrowth in differentiated SH-SY5Y cells", *Cell communication and signaling*, 2021, **18**, 118.
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5. Badr Jismy, Abdelkarim El Qami, Anja Pišlar, Rok Frlan, Janko Kos, Stanislav Gobec, Damijan Knez, Mohamed Abarbri, "Pyrimido[1,2-b]indazole derivatives: selective inhibitors of human monoamine oxidase B with neuroprotective activity", *European journal of medicinal chemistry*, 2021, **209**, 112911.
6. Tina Vida Plavec, Tim Ključevšek, Aleš Berlec, "Introduction of modified bglbrick system in *Lactococcus lactis* for straightforward assembly of multiple gene cassettes", *Frontiers in bioengineering and biotechnology*, 2021, **9**, 797521.
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8. Milica Perišić, Graham Pawelec, Janko Kos, "Human CD4+ T-cell clone expansion leads to the expression of the cysteine peptidase inhibitor cystatin F", *International journal of molecular sciences*, 2021, **22**, 16, 8408.
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10. Spase Stojanov, Tina Vida Plavec, Julijana Kristl, Špela Zupančič, Aleš Berlec, "Engineering of vaginal lactobacilli to express fluorescent proteins enables the analysis of their mixture in nanofibers", *International journal of molecular sciences*, 2021, **22**, 24, 13631.
11. Mirjana Malnar, Boris Rogelj, "SFPQ regulates the accumulation of RNA foci and dipeptide repeat proteins from the expanded repeat mutation in C9orf72", *Journal of cell science*, 2021, **134**, 4, jcs256602.
12. Janko Ignjatovic, Nevena Đajić, Jovana Krmar, Ana Protić, Borut Štrukelj, Biljana Otašević, "Molecular docking study on biomolecules isolated from endophytic fungi", *Journal of the Serbian Chemical Society*, 2021, **86**, 2, 125-137.
13. Tina Vida Plavec, Ana Mitrović, Milica Perišić, Borut Štrukelj, Janko Kos, Aleš Berlec, "Targeting of fluorescent *Lactococcus lactis* to colorectal cancer cells through surface display of tumour-antigen binding proteins", *Microbial biotechnology*, 2021, **14**, 5, 2227-2240.
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15. Wouter van Rheenen *et al.* (247 authors), "Common and rare variant association analyses in amyotrophic lateral sclerosis identify 15 risk loci with distinct genetic architectures and neuron-specific biology", *Nature genetics*, 2021, **53**, 12, 1636–1648.
16. Ana Dolšak, Tomaž Bratkovič, Larisa Mlinarič, Eva Ogorevc, Urban Švajger, Stanislav Gobec, Matej Sova, "Novel selective IDO1 inhibitors with isoxazolo[5,4-d]pyrimidin-4(5H)-one scaffold", *Pharmaceuticals*, 2021, **14**, 3, 265.
17. Ilona Bereczki *et al.* (21 authors), "Natural apocarotenoids and their synthetic glycopeptide conjugates inhibit SARS-CoV-2 replication", *Pharmaceuticals*, 2021, **14**, 11, 1111.
18. Spase Stojanov, Matjaž Ravnikar, Aleš Berlec, Samo Kreft, "Interaction between silver fir (*Abies alba*) wood water extract and lactobacilli", *Pharmazie*, 2021, **76**, 12, 614-617.
19. Samo Kreft, Borut Štrukelj, "Influence of magnesium sulphate on cholecystokinin, hunger, and obesity", *Progress in nutrition*, 2021, **23**, 3, 9081.

Review Article

1. Valentina Novak, Boris Rogelj, Vera Župunski, "Therapeutic potential of polyphenols in amyotrophic lateral sclerosis and frontotemporal dementia", *Antioxidants*, 2021, **10**, 8, 1328.
2. Anja Pišlar, Lara Bolčina, Janko Kos, "New insights into the role of cysteine cathepsins in neuroinflammation", *Biomolecules*, 2021, **11**, 12, 1796.
3. Kawaljit Kaur, Meng-Wei Ko, Anahid Jewett, Po-Chun Chen, Barbara Breznik, Emanuela Senjor, Paul Wong, Yuhao Wang, Nishant Chovatiya, "Probiotics in health and disease: distinct roles of different strains in natural killer cell activation and regulation", *Critical reviews in immunology*, 2021, **41**, 2, 1-19.
4. Tanja Jakoš, Anja Pišlar, Anahid Jewett, Janko Kos, "Myeloid-derived suppressor cells hamper natural killer cell activity in cancer: role of peptidases", *Critical reviews in immunology*, 2021, **41**, 2, 77-99.

5. Milica Perišić, Urša Pečar Fonović, Tanja Jakoš, Janko Kos, "The role of cysteine peptidases in hematopoietic stem cell differentiation and modulation of immune system function", *Frontiers in immunology*, 2021, **12**, 680279.
6. Ana Rotter *et al.* (61 authors), "The essentials of marine biotechnology", *Frontiers in marine science*, 2021, **8**, 629629.
7. Nikolaja Janež, Blaž Škrlj, Meta Sterniša, Anja Klančnik, Jerica Sabotič, "The role of the Listeria monocytogenes surfactome in biofilm formation", *Microbial biotechnology*, 2021, **14**, 4, 1269-1281.
8. Helena Motaln, Nina Recek, Boris Rogelj, "Intracellular responses triggered by cold atmospheric plasma and plasma-activated media in cancer cells", *Molecules*, 2021, **26**, 5, 1336.

Independent Component Part or a Chapter in a Monograph

1. Borut Štrukelj, "From gene engineering to modern biologicals", In: *Course notes. 4, Drug design, advanced therapy medicinal products and microbiology*, Ljubljana Faculty of Pharmacy, 2021, 95-123.
2. Janko Kos, Anahid Jewett, Anja Pišlar, Tanja Jakoš, Emanuela Senjor, Milica Perišić, "The role of peptidases and their endogenous inhibitors in the regulation of NK cell cytotoxicity", In: *Successes and challenges of NK Immunotherapy: breaking tolerance to cancer resistance*, Academic Press, 2021, 83-100.
3. Anahid Jewett, Janko Kos, Tamara Lah Turnšek, Po-Chun Chen, Barbara Breznik, Emanuela Senjor, Nishant Chovatiya, Kawaljit Kaur, Meng-Wei Ko, "Novel strategies to expand supercharged NK cells with augmented capacity to withstand inactivation by tumors", In: *Successes and challenges of NK Immunotherapy: breaking tolerance to cancer resistance*, Academic Press, 2021, 101-119.

Encyclopaedia, Dictionary, Lexicon, Manual, Atlas, Map

1. Jernej Šribar, Jerica Sabotič, *Navodilo za delo z ultracentrifugo Beckman Coulter Optima XPN-90: poslovna tajnost*, Institut Jožef Stefan, 2021.

Patent Application

1. Mojca Lunder, Borut Štrukelj, Peter Korošec, Ana Koren, *IgE epitope-like peptides and uses thereof*, US2021115097 (A1), US Patent Office, 22. 04. 2021.

Theses and Mentoring

1. Tina Vida Plavec, *Surface display of tumor antigen binders on Lactococcus lactis NZ9000 and evaluation of their binding to selected human tumor cell lines:* doctoral dissertation, Ljubljana, 2021 (mentor Aleš Berlec; co-mentor Borut Štrukelj).

DEPARTMENT OF ENVIRONMENTAL SCIENCES

The Department of Environmental Sciences focuses on the interweaving of the physical, chemical and biological processes that shape our environment, the human and its activities. Our research is interdisciplinary and multidisciplinary and takes place in several areas, such as environmental analytical chemistry, biogeochemical cycles, microbial ecology, environment and health, environmental technologies, risk and environmental assessment, and environmental monitoring. We also work on the development of technical solutions for environmental problems and environmental management. The department hosts the "ISO-FOOD" ERA Chair for isotope techniques in food safety, quality and traceability, the infrastructure Centre of Mass Spectrometry (CMS) and the Mobile Ecological Laboratory Unit (ELME).

Head:
Prof. Milena Horvat

Analytical chemistry of the environment and biological systems

Inorganic

The role of trace elements and their impact on the environment and living organisms depend on both their total concentration and the chemical forms in which they are present. Our research is focused on the development of new analytical procedures for the speciation of elements like Al, As, Cr, Se, Sn, Br, Pt, Ru, Ni, V, Zn, etc., in environmental, food and biological samples.

In the field of *elemental speciation*, conjoint liquid chromatography (CLC) was used for the separation of Cu bound to ceruloplasmin (Cp) and albumin (HSA) in human serum. Two immunoaffinity CIMac albumin depletion (anti-HSA) disks and one CIMac weak anion-exchange diethylamine (DEAE) disk were assembled in a single housing forming a CLC monolithic column. HSA was retained by the anti-HSA disk, enabling a subsequent separation of Cu bound to low-molecular-mass (LMM) ligands, from Cu bound to Cp. Finally, the Cu associated with HSA was eluted from the column. The separated Cu species were quantified by post-column ID-ICP-MS. The developed method will be applied in the analysis of Cp in real human-serum samples.

A new analytical method for the speciation of Cr-LMM complexes and Cr(VI) in plants using anion-exchange HPLC-ICP-MS was developed. Cr-binding ligands were identified by HR-MS. The developed method was applied in the Cr speciation of dandelions growing in soil with a high Cr content and in a study of the uptake and transformation of Cr species in dandelion plants exposed to Cr(VI) or Cr-nitrate. Localization of Cr in a dandelion leaf was performed with laser ablation (LA)-ICP-MS. Our research makes an important contribution to understanding the transport, metabolism and detoxification processes of Cr in plants and the knowledge that can be used in planning effective remediation strategies using plants.

In the field of bioimaging of metal ions we continued with the optimization of the parameters for the LA and quantification of an ablated sample with ICP-MS in tumour spheroids and plant tissue, with the aim to achieve high spatial resolution and low limits of detection.

Organic

We synthesised a molecularly imprinted polymer (MIP) with the aim to extract an active pharmaceutical substance bupivacaine from blood-derived samples. While at higher concentrations this material showed promising results, the leaching of the template from the material makes the method ill-suited at lower levels. This was solved by replacing the template with a structurally similar analogue as a part of the MIP synthesis procedure.

A reference solid-phase extraction method was developed and validated for the local anaesthetic drug bupivacaine and sedative dexdemetomidine in plasma samples. The method was then used for pharmacokintetics studies of anaesthetized dogs after a single intravenous or perineural administration of the drugs. Such studies are important in the context of improving the pain management for dogs following a tooth extraction.

The analytical method for the determination of bleomycin in blood-derived and tumour samples was optimized, simplified and revalidated. In this frame, novel extraction materials were included and the extraction was transferred to a positive-pressure 96-well-plate extraction system. In the context of validation, the stability of the analyte in
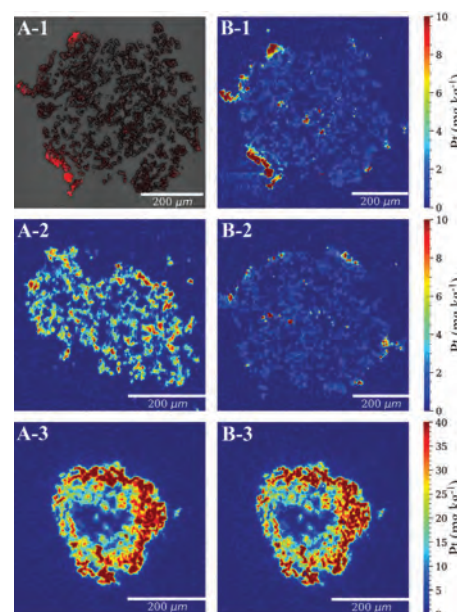
Figure 1: High spatial resolution imaging of cisplatin and Texas Red cisplatin in tumour spheroids using laser ablation isotope dilution inductively coupled plasma mass spectrometry and confocal fluorescence microscopy
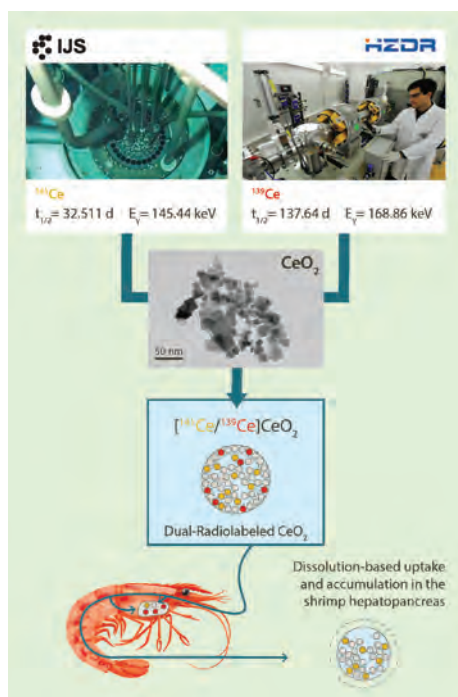
Figure 2: Analysis of complex environmental processes via cross-institute, cross WP complimentary facility use

different matrices was examined and a quality-control system was established. The method was further adapted for the determination of bleomycin at trace-level concentrations in in vitro systems.

A non-target screening approach was used to investigate the biodegradation of two bisphenols, i.e., BPF and BPS, during biological wastewater treatment with activated sludge. Both compounds followed first-order kinetics. In addition, four biotransformation products (one novel one) of BPF and eleven (ten new) BPS transformation products were identified. The data also support possible new biodegradation pathways, namely sulphation, methylation, cleavage and the coupling of smaller bisphenol moieties.

We also examined the toxicity of BPA, BPF and their binary mixture towards primary producers. The results demonstrated that prokaryotic cyanobacterium *Synechococcus leopoliensis* is is more sensitive than eukaryotic green alga *Pseudokirchneriella subcapitata*, whereas the toxic potentials of the two BPs are comparable, indicating a comparable hazard for phytoplankton. When the mixtures were tested, an additive effect was observed in *P. subcapitata* over the whole concentration-range effect, whereas for *S. leopoliensis*, no pronounced combined effect was observed. However, more data on the toxicity to aquatic species, including their combined effect, and the data on their occurrence in the aquatic environment are needed to enable a full environmental risk assessment.

Metrology

Metrology – the science of measurement – is crucial for the department as most research is related to measurement or the use of measurement results. The department is the institute designated to develop the national metrology system identifying the amounts of substances, particularly of trace elements in organic and inorganic materials.

Metrology in a traditional stable isotope analysis of light elements covers: (i) development of new reference materials for the environment including greenhouse gasses such as CO_2 and CH_4 as a part of the EMPIR STELLAR project, and evaluation of the measurement uncertainties in these materials; and (ii) participation in the interlaboratory comparisons at the highest metrology level. In 2021 we participated in the evaluation of results in the CCQM-167 interlaboratory comparative scheme Carbon Isotope Delta Measurements of Vanillin and in the implementation of analyses under CCQM-204: Pilot Study on CO_2. We prepared minimum criteria for reporting HCNOS isotopic delta values as a result of a virtual technical meeting organized by the IAEA entitled *Development of reference materials for stable isotopes and related products*.

The department is also actively involved in two metrology-related networks: ESFRI Infrastructure for the Promotion of Metrology in Food and Nutrition (METROFOOD-RI) where the JSI acts as the coordinator of the Slovenian Joint

Figure 3: Occurrence, treatment, removal and transformation of contaminants of emerging concern (CEC)

Research Unit and in the preparation of a new network within the EMPIR program (European Metrology Program for Innovation and Research) called FoodMetNet, started in June 2020, supporting the joint European research in the field of food safety and sustainability.

Within projects MercOx, SI-Hg and GMOS-train we focused on the metrology of atmospheric Hg species. The existing metrological infrastructure for atmospheric Hg speciation was evaluated and the focus was on the most problematic parts of the analytical procedure: sampling, preconcentration methods and calibration. Sampling/preconcentration using sorbent traps, sorbent membranes, impinging solutions and denuders were tested and according to the validation experiments, they were found either as suitable or unsuitable for atmospheric Hg speciation. Similar validation experiments were also performed for the calibration methods such as evaporative calibrators, bell-jar calibrators and batch-type calibrators. In addition to well established Hg analytical procedures (such as cold vapour atomic fluorescence/absorbance – CV AFS/AAS), validation was also performed with [197]Hg radiotracer, enabling ambient level concentration experiments due to its specificity and selectivity. To complement the evaluation of the existing calibration methods, we developed our own calibration for gaseous oxidized mercury (Hg^{II}) species. The newly developed calibration was based on non-thermal plasma oxidation of elemental mercury (Hg^0) to Hg^{II} species (HgO, $HgCl_2$ and $HgBr_2$) in the presence of a reaction gas. Due to the quantitative oxidation and traceable amount of Hg^0 we generated the first SI-traceable amounts of Hg^{II} species at ambient concentration levels. Our work done on the metrology of atmospheric
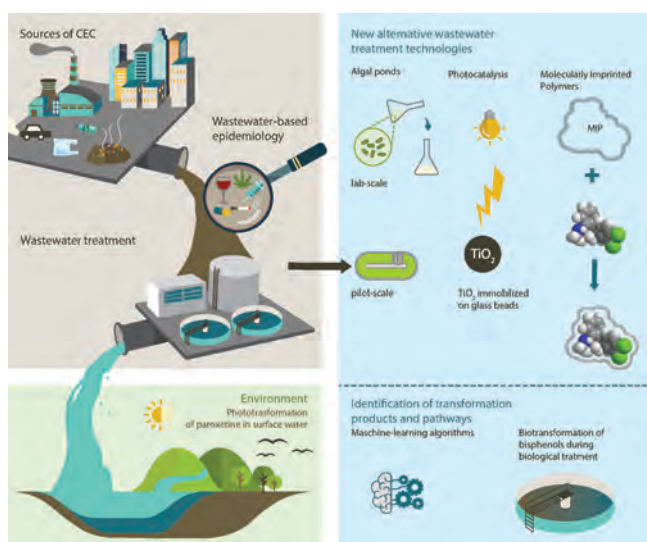
Hg species greatly contributed to the potential achievement of comparability and could provide much needed trust in the worldwide measurement data.

Biogeochemistry and climate change

In collaboration with Velenje Coal Mine d.o.o., we investigated the degassing mechanisms and the genesis of the coal gas trapped in lignite at the active excavation fields in the Velenje Coal Basin. Based on carbon-isotope compositions of CO_2 and methane, a predominantly biogenic origin of both gases was confirmed, where the proportions of biogenic and geogenic fractions showed some spatial variability.

In the study of the terrestrial CO_2 cycle, river carbonates as a potential CO_2 sink were investigated using the isotope ratios of uranium ($^{234}U/^{238}U$ activity ratio) and strontium ($\delta^{88}Sr$ value) in river sediments as the identifiers of authigenic carbonate. We were able to show that not only identification, but also quantification of the CO_2 fixation rate is possible, provided that the local end-members (water, soil, bedrock) and the spatial variability of their U and Sr isotope compositions are known.

The susceptibility and symptoms of eutrophication in the Chesapeake Bay (CB) and Northern Adriatic Sea (NAS) were compared. The study also discusses recent reversals of eutrophication (oligotrophication) and future considerations. The differences in the residence time of water (CB > NAS), volume relative to the riverine transport of nutrient-rich water (CB << NAS), bathymetry, freshwater-driven seasonal stratification, and density-driven estuarine circulation make the CB more susceptible to eutrophication than the NAS. It is also important to note that NAS has a high buffer capacity due to the riverine input of the carbonates dissolved from Alpine and Karstic watersheds, and its waters should have a higher resilience to acidification. In shallow eutrophic areas, the combined effect of the rising atmospheric CO_2, warming and river-induced anthropogenic CO_2 with the associated decrease in the buffer capacity can lead to an acidification process. A significant effect on calcifying organisms is expected in the future.

Within the CRP project *Identification of Pb sources in the Upper Mežica Valley*, we determined the sources of Pb in the environment on the basis of its isotopic composition. Environmental samples, such as the water and sediments of the Meža River and its tributaries, and most soil samples from the valley have an isotopic composition of Pb that matches that of the local Pb ores (galena and wulfenite). It is different with dust (PM_{10}) particles. The isotopic composition of Pb in them coincides with that found in the battery produced at the local battery factory.

We started new research – monitoring the occurrence and transformations of microplastics and nanoplastics in natural systems. For this purpose we are developing sensitive analytical methods for determining the concentration and sizes of microplastics and nanoplastics in environmental matrices and at environmentally relevant (low) concentrations. Using the method based on inductively coupled plasma mass spectrometry in the single-particle mode (SP-ICP-MS), we are also studying the type and concentration of potentially toxic elements present in microplastics, either in the form of additives or in the form of contaminants adsorbed on the surface.

Figure 4: Improving the metrology of atmospheric HgII species

Within the Danube Hazard m3c project, selected elements from the river water, wastewaters and atmospheric deposition samples were collected at 20 sampling sites alongside the Danube River Basin and measured. Different types of inorganic nanoparticles (NPs containing Ti, Ce, Pb, Cr, Mn, Fe, Cu, Zn, etc.) were also identified and their concentration as well as particle-size distribution in the river water samples were quantified.

In the framework of the CROSSING project and in collaboration with the HZDR we developed an innovative dual-radiolabelling strategy for CeO_2 nanoparticles using neutron activation and in-diffusion labelling to radiolabel CeO_2 nanoparticles with both Ce-141 and Ce-139. Varied distribution of radiolabels in the particles does not only allow an easy dose determination in the uptake studies but also enables us to track the uptake pathways of the anthropogenic cerium as shown with an example of a freshwater shrimp. The results suggest a dissolution-based translocation of cerium over the gut wall and a consequent exposure of the internal organs of the crustaceans to potentially toxic, dissolved cerium species. This has further implications for the fate of anthropogenic cerium in the environment and its potential accumulation in the food chain.

Water cycle

In the framework of a Slovenian-Hungarian bilateral collaboration and long-term cooperation with the IAEA, a detailed geostatistical assessment of the spatial representativity of stations in two national monitoring networks of isotopes in precipitation was performed. The under- and over-represented areas were identified and the importance of data exchange with the neighbouring countries was emphasised. In the field of urban hydrology, the mixing of water from different pumping stations in the Ljubljana water supply system was traced using stable water isotopes.
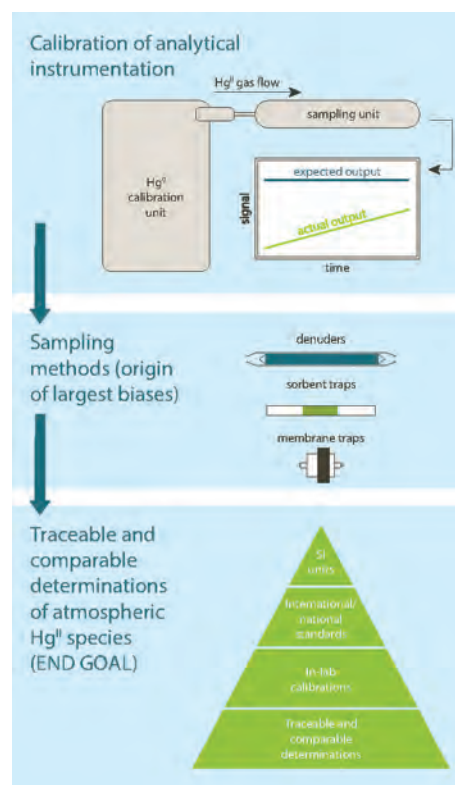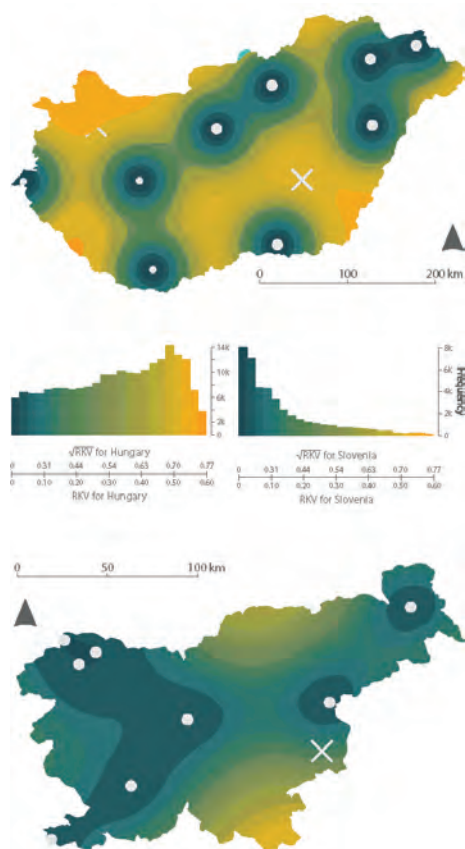
Figure 5: Optimisation of monitoring networks of O and H isotopes in precipitation in Slovenia

Monthly monitoring, sampling and measurements of Hg and different water parameters on the Idrijca and Soča Rivers continued on six locations on both rivers. Pilot sampling in the Gulf of Trieste was also performed and it will be the subject of further research. Even 25 years after the closure of the Hg Mine in Idrija, the Soča River brings considerable amounts of Hg into the Gulf; however, the species of Hg depends on the location, environmental conditions and biogeochemical processes that occur in the river and gulf. Work is done within the project *Innovative isotopic techniques for identification of sources and biogeochemical cycling of mercury in contaminated sites – IsoCont*.

The research on Hg in air continued at different locations in Slovenia. In Deskle, a town that is in the influence area of the Anhovo cement plant, a whole-year monitoring of Hg in air was performed for the Slovenian Environmental Agency. Monitoring for the same agency was also performed at the Iskrba meteorological measurement station that is considered as a pristine area. At Iskrba, precipitation samples are also collected.

In cooperation with Aerosol d.o.o., the measurement of Hg speciation in Ljubljana air was performed.

Air

Our research on the ambient-air quality in Ljubljana was continued, using continuous radon monitoring in outdoor air to classify the atmospheric stability and determine the atmospheric boundary layer. The study was conducted in cooperation with the Aerosol company within the STRAP project (Sources, transport and fate of persistent air pollutants in the environment of Slovenia).

In the indoor air quality research, our attention was focused on the ventilation efficiency in buildings with increased airtightness after the energy renovation where the indoor/outdoor air exchange rate is often insufficient. The ventilation efficiency was tested by simulating the radon concentration in the air of a classroom at a primary school, in which, after the energy renovation, the measured radon concentration exceeds the limit of 300 Bq m^{-3} by a factor of two or three. In the simulation, we considered 25 ventilation cases (taking into account 15 scenarios with the design ventilation rates (DVRs), covered by international and national regulations and recommendations) and found that in 6 cases (24 %) DVRs were insufficient according to the EU guidelines and in 14 cases (56 %), they were insufficient according to the WHO guidelines. In collaboration with the Faculty of Mechanical Engineering and the Faculty of Civil and Geodetic Engineering, we carried out the research project *Expert opinion on the adequacy of ventilation of the Faculty of Law, the University of Ljubljana, to prevent the spread of coronavirus (SARS-CoV-2)*.

As part of the RI-SI-EPOS infrastructure project we obtained several up-to-date portable monitors to detect the activity concentration of radon and thoron and their products in various media.

Colloid biology

In 2021 the main research activities were carried out under two European research projects:
– EC program H2020 funded SURFBIO project (Innovation hub for surface and colloid biology research)
– EC program H2020 funded GREENER project (InteGRated Systems for Effective ENvironmEntal Remediation)

Within the SURFBIO project (Twinning funding scheme) we built up a consortium of research partners, from which the JSI is transferring the knowledge to boost its expertise in surface and colloid biology research. Together with the partners, we have started to build a research hub, which will address the basic scientific questions and provide the solutions for applicative problems in different industries.

Within the GREENER project we implemented the methods for combining cells into artificial multi-cellular structures, i.e., aggregates and biofilms, by "gluing" them together and to the surfaces of particles or onto larger surfaces of different materials. The constructed 2D and 3D structures were of different compositions, sizes and thicknesses. Based on these methods, we were able to show in vitro the importance of the proximity between two bacterial cells exchanging nutrients between each other. A patent application of this innovative approach filed in 2020 was approved in 2021 and the technology received a Bronze Medal and ARCA 2021.

By combining different bacteria into artificial structures, metabolic coupling can be performed for different solutions applicative to medicine, biotechnology and environmental bioremediation sciences. This study was carried out as part of the international project ARRS N1-0100 BE MERMAiD – *Bioavailable mercury methylation in the Adriatic Sea* where several experiments with constructed artificial biofilms on surfaces have shown promising

results for the reduction and precipitation of toxic metals. The artificial structures and their characteristics were published in the journal Frontiers in Materials.

Within the CROSSING international project (a collaborative research project between the JSI and Helholz-Zentrum Dresden-Rosendorf – HZDR, Germany, funded by HZDR) we further analysed the interactions between bacteria and nanoparticles, as well as bacteria and metal surfaces with different physical characteristics obtained by nanoprinting and etching. Our collaboration activities also resulted in a publication in the journal Environmental Science: Nano.

Together with the group for radiochemistry, we continued our work in the frame of the national project *Cost-efficient separation of tritium from water with bio-based systems* – BIOTRISEP (ARRS J7-2597). We carried out preliminary experiments for the tritium separation using cyanobacteria to show a preliminary proof of concept of the bio-based approach. In two other

Figure 6: Wastewater remediation approaches and artificial biofilms on material surfaces

national projects (ARRS J1-9194, ARRS J3-1762) we were collecting and characterizing bacterial isolates from the oral cavity and the skin surface of babies and started characterizing their antimicrobial activities. We also started sequencing and annotating the genomes of the selected bacterial isolates.

In collaboration with the Chemical Institute we prepared a system for the purification of different organic pollutants used in paper making, which was based on a bacterial immobilization system, and demonstrated the proof-of-concept for such a purification system. The work was published in Frontiers in Microbiology.

Environment and health

In collaboration with the Faculty of Health Sciences, University of Ljubljana we investigated the causation of oxidative stress and defence response of a yeast-cell model after a treatment with orthodontic alloys consisting of metal ions. In collaboration with the Faculty of Electrical Engineering, University of Ljubljana we investigated the metal release from the electrodes used in electroporation with nanosecond pulses and cisplatin.

We continued with arsenic speciation in human biomonitoring samples and found that urine samples from children from the Upper Mežica Valley contained slightly more dimethylarsenic acid than is usual for the samples from other areas. Concentrations of total arsenic were still below the limit ($<15 \, \mu g / L$). In the HBM4EU project, we performed a risk assessment for inorganic arsenic in the general European population. Due to the low concentration of arsenic in drinking water in most of Europe, the exposure is low and, taking into account the latest studies on the mechanism of the actions of inorganic arsenic at low concentrations, the risk to the general population is very low.

We continued with the field work within the national HBM program (HBM2018-23), which deals with a chemical-exposure assessment of children (6–9 years) and teenagers (12–15 years). Due to the Covid-related restrictions, we had to modify the sampling campaign, which took place at the Reactor Centre and not at the primary schools in the selected study areas as in the pre-Covid period. Consequentially, the number of recruited children and teenagers was smaller than expected, but we successfully completed the collection of human samples and questionnaire data relating to the selected groups of children and teenagers in Vrhnika. The samples collected in 2020 in other study areas were analysed for elements, bisphenols, parabens, triclosan, polycyclic aromatic hydrocarbons (PAH) and phosphorous flame retardants.

We also continued with the recruitment of pregnant women and sample collection during their pregnancy, at birth and postnatally from the Celje Region in collaboration with the Celje Maternity Hospital. By the end of 2021, 68 pregnant women were recruited.

The data analysis and interpretation of the results from the previous HBM studies, mostly from the first national HBM programme, resulted in three publications covering the exposure of men and lactating women to environmental phenols, phthalates and DINCH (Chemosphere), and a further assessment of susceptibility to phthalate, DINCH exposure through CYP and UGT single nucleotide polymorphisms (Environment International), and exposure to PAHs in men and lactating women in Slovenia (International Journal of Hygiene and Environmental Health). The overall work identified important sources of exposure to relevant chemicals (consumer products, different environmental sources), behaviour-related exposure and geographic variability across Slovenia as well as the genetic factors that have a role in the biotransformation of specific substances, therefore influencing the exposure and susceptibility to these substances.

At the European level and within the HBM4EU project we performed a risk assessment of arsenic and initiated a risk assessment of inorganic mercury. We also continued with the assessment of geographic variability of cadmium across Europe, exploring the dietary-related differences between different countries and regions of Europe. In 2021, new data on the exposure to priority substances was generated within the project (aligned studies data), part of which was also the Slovenian study of children and adolescents from Prekmurje, conducted as a pilot study within
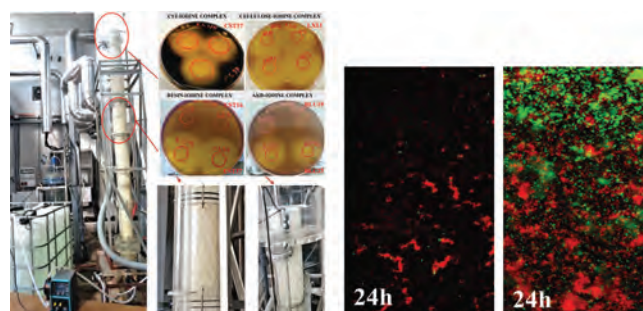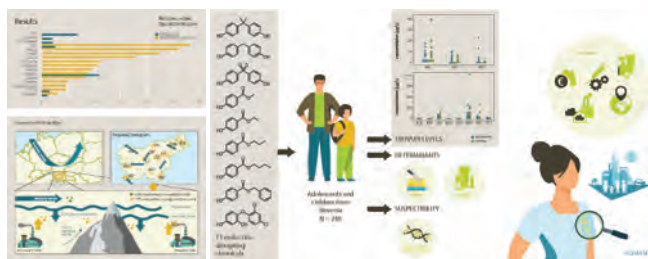
Figure 7: Human biomonitoring in the context of environmental and human-health interactions

the national HBM programme. For the Slovenian population, phosphorous and brominated flame retardants, and perfluorinated compounds were additionally determined using the co-funding from the project. A data analysis of these substance groups was initiated at the European and national level in order to assess the exposure levels, identify determinants of exposure and explore geographic variability.

We developed and validated the workflow for suspect and non-targeted screening of exposure biomarkers in human urine. This workflow included the sample preparation, instrumental analysis and data processing procedures. It was then applied as a proof-of-concept to identify the biomarkers of exposure in urine of a cohort of 200 children from Slovenia, aged 6–9 years. The analysis revealed 76 biomarkers of exposure from several classes of pharmaceuticals, personal care products, plasticizers, pesticides, etc. The results shed light on simultaneous exposures of Slovenian children, opening up questions on a potential adverse effect of such mixtures on this vulnerable population.

Wastewater-based epidemiology can provide objective and reliable data on spatio–temporal licit and illicit drug-use patterns. In our study, we used a wastewater analysis to investigate drug prevalence in Slovenian educational institutions regarding the level of education (primary, secondary and higher education), geographic location (inter-municipality comparison) and degree of urbanization (urban vs non-urban areas). The results showed that the residues of drug abuse were present in all samples, while residues of nicotine, alcohol and cannabis were detected most frequently. The study confirmed that drugs are present in young people's lives already in the early stages of their education, and that the educational level of an institute influenced consumption patterns the most. In addition, we were also involved in an international study regarding the identification of new psychoactive substances in several European populations assessed by wastewater-based epidemiology. The results showed that this approach is valuable, following rapidly the changing profiles of use.

Nanomaterials and biosensors

In collaboration with the National Chemical Institute, Ljubljana, Slovenia, and the Hebrew University of Jerusalem, Israel, we reported on the deposition, testing and antioxidation properties of ultra-thin (1–3 nm) mono-, di- and tri-layer hybrid organic-inorganic polyhedral oligomeric silsesquioxanes (POSS) on Inconel 617. We envision that such coatings will have significant potential as primers for spectrally selective absorber coatings used for the concentrated solar power (CSP) hybrid absorber technology. Our collaboration activities also resulted in a publication in Solar Energy Materials and Solar Cells.

The production, synthesis, characterization, scaling-up and properties of 2D nanomaterials were also studied under different international and national projects: MercOx (Metrology for oxidized mercury; 16ENV01) funded under EMPIR (The European Metrology Programme for Innovation and Research), H2020 ERA-NET Cofund, GA689443 ERA-PLANET/IGOSP, ARRS N1-0100, P1-0143 and J1-1716. The findings were been published in Nanoselect.

We also collaborated with the Electronic Ceramics Department (K5) to develop nanomaterial thin and thick films using screen-printed methods on two different substrates (Al_2O_3 and LTCC) and utilize them as transducer-based biosensor platforms for the detection of different targeted analytes.

The head of the department is also involved with the group for radiochemistry and colloid biology through the national project *Cost-efficient separation of tritium from water with bio-based systems* – BIOTRISEP (ARRS J7-2597).

We collaborated with the National Institute of Animal Biotechnology (NIAB), India, to work on electrochemical-based biosensors for SARS-CoV-2 and cancer research. Within this work, we prepared peptides and bioconjugates to target cancer cells and develop strategies to immobilise biomolecules on nanomaterials. The above activities resulted in publications in journals Frontiers in Immunology and Cancers.

Food/nutrition including ERA Chair Isofood

In samples of milk, cheese, feed and water from Greece we determined the multi-element composition and isotopic ratio of $^{87}Sr/^{86}Sr$ in order to characterize local products from different parts of Greece. We also determined which parameter (milk, water or feed) influences the most the isotopic composition of cheese. In order to determine the geographical origin of hemp, we determined the isotopic composition of Sr in hemp tops, roots and soil for the samples from different parts of Italy.

The use of stable isotopes of light and heavier elements were used for:

Identification of the geographical origin of Slovenian milk. The study shows that the $^{87}Sr/^{86}Sr$ ratios can be a powerful tool for determining the geographical origin of food originating from the countries with more homogenous geology, while any interpretation based on the $^{87}Sr/^{86}Sr$ ratios can be challenging for the countries with heterogene-

ous geology, such as Slovenia and many other EU countries. On the other hand, as a tool for investigating a broader geographical origin, the strontium method is very useful, but it does require detailed knowledge of the geology and the land use. Further, the $^{87}Sr/^{86}Sr$ ratios can become more useful for the geographical origin discrimination if combined with the stable isotopes of light elements and elemental composition.

Differentiation between natural and synthetic aroma compounds. The IsoVoc database was constructed and used for the authentication of natural flavours. In total, 25 aroma compounds were identified and used to test 33 flavoured commercial products to evaluate the usefulness of the IsoVoc database for the fruit flavour authenticity studies. The results revealed a possible falsification for several fruit aroma compounds.

Identification of the type of production (organic vs. conventional). We examined the difference in the content of prenylflavonoids in hops and beer produced under organic and conventional production regimes and combined them with the $^{15}N/^{14}N$ and $^{13}C/^{12}C$ isotope ratio analysis. The results show no statistical difference in the content of the selected prenylflavonoids between the organically and conventionally produced hopes and beer. The stable-isotope analysis indicated that only the $\delta^{15}N$ values are statistically higher in organically produced hops and beer. However, the differentiation according to the type of production could not be made solely based on the $\delta^{15}N$ signature, but it could be used to provide supporting evidence.

The characterization of new alternative food sources focusing on algae was performed. The studies included: (i) identification of the types of extremophiles in the moderate climate of Central Europe, in particular in Slovenia, and their potential use in biotechnology and bioremediation applications; (ii) characterization of the algae dietary supplements obtained on the Slovenian market using antioxidative potential, elemental composition and stable isotope approach; and (iii) investigation of the antioxidant effect of fermented and non-fermented Spirulina extracts on the proteome level, using the yeast *Saccharomyces cerevisiae* as the model organism. We began to investigate the farmed insects for food and feed under the INPROFF: Quality, Safety and Authenticity of Insect-Protein Based Food and Feed project.

The obtained data on the investigated food commodities are also included in the e-components of different EU projects such as METROFOOD-RI and FNS-Cloud. In 2021 the expert task of checking the origin of apples and olive oil and establishment of the database of Slovenian honey samples was performed for the Administration of the Republic of Slovenia for Food Safety, Veterinary and Plant Protection. In 2021 the new MSCA ITN FoodTraNet: Advanced Research and Training Network in Food quality, safety and security (FoodTraNet) project, coordinated by Nives Ogrinc, was started. The goal is to train and mobilize 15 early-stage researchers to develop advanced methods for maintaining food quality, authenticity and traceability, and create radical food production and safety solutions, using advanced materials and technologies. Information is available at https://www.foodtranet.org.

Figure 8: Acquisition of the MSCA ITN Foodtranet in conjunction with ERA-Chair IsoFood, successfully operating in the field of safe and healthy food

Environmental technologies

We continued research on cement-organic-radionuclide interactions for a safe disposal of low- and intermediate-level radioactive waste within the framework of work package CORI of the EURAD H2020 European Joint Programme on Radioactive Waste Management. We studied radiolytic and hydrolytic degradation of a commercial polycarboxylate superplasticizer intended to be used as an additive to concrete for radioactive-waste disposal purposes. The results show that after prolonged irradiation to 3.2 MGy and/or hydrolysis, samples are degraded to polyethylene glycol, which is cleaved off the backbone.

The influence of artificial aeration on the sludge decomposition process in mesocosm sludge treatment reed beds (STRBs) was investigated. In addition to the typical STRB design, where ventilation is mainly provided by a drainage pipe, passive aeration via a "chimney" and active aeration via a blower were introduced. The results indicated an accelerated sludge degradation process in both active and passive beds. However, this effect was limited to part of the season and could not be demonstrated by episodic measurements of CO_2 efflux. Isotopic analyses revealed changes in decomposition dynamics for certain parts of the season, differences in the contributions of sludge and plant derived CO_2 to the total CO_2 emissions from differently aerated beds. Overall, passive aeration proved to be similarly efficient as active aeration and could therefore be considered for application in a full-scale system.

Environmental management, environmental impact assessment and risk assessment

In 2021 we continued the activities within the TransCPEarlyWarning project, which aims to improve the level of coherence of the existing civil protection early warning, in order to increase the capacity to anticipate, warn and
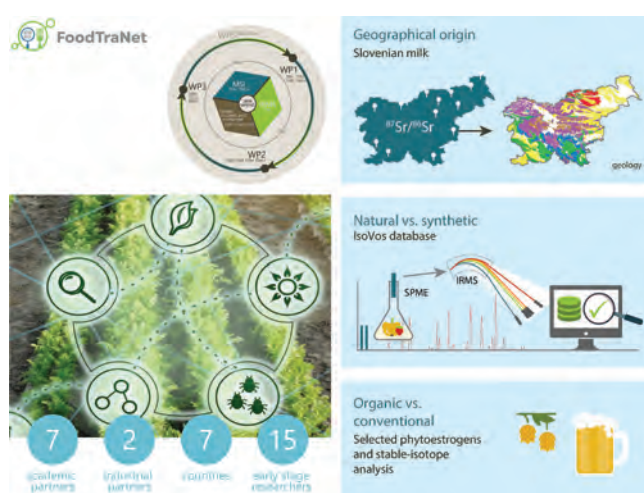
respond to threats and improve information exchange and coordination with the EU civil-protection mechanism and risk management. Specifically, this refers to increasing uniformity and homogeneity through the integration of the existing early-warning approaches, thus improving the exchange of information within the European Civil Protection Mechanism. The work consisted of the finalisation of the preparatory work for the modelling phase for floods and wildfires to be used in the development of the common early-warning platform, to help harmonise and improve the detection of risks and related emergency response. Data collection, management and analyses were performed for the partner countries with the aim of generating a clear picture about the current state-of-the-art regarding the civil protection and early-warning systems.

We participated in the HERA project (Health and Environment Research Agenda, HERA Integrating Environment and Health Research: a Vision for the EU 2019–2022). The purpose of the HERA project was to set research priorities in the field of environment, climate and health in the EU. This research intended to guide decision-making and help achieve the ultimate goals of protecting and improving the quality of the environment and human health. Through a holistic, systematic and inclusive approach, project partners and stakeholders identified opportunities to improve health and highlight important environmental issues that urgently need to be addressed. People are increasingly concerned about the deteriorating state of the environment and the associated health effects. Biodiversity loss, environmental pollution and exposure to harmful substances can be detrimental to health and reduction of quality of life. The impact on the socially disadvantaged and vulnerable is also of particular concern.

The aim of the project was to identify the key orientations for future research, strategies and tools to address environmental, climate and health issues, taking into account identified societal needs, related sectoral policy objectives and knowledge gaps in the field. This was achieved by establishing effective communication between the stakeholders at the national and European levels, i.e., by involving stakeholders, developing additional guidelines for the health impact assessment and health risk assessment, increasing coordination and enrichment of ideas, and contributing to the European policy and practice.

Within the NEUROSOME project, we were focused on addressing the alerts about the unclear role of health risk assessment (HRA) in informing about public health decisions; we explored the understanding of HRA and its results in the decision-making context. A survey was conducted among different stakeholders showing various understandings of HRA, which seem to be the reason for the inconsistency within the HRA realm, ultimately resulting in a loss of its effectiveness and primary purpose: to inform about public health decisions. As a result of this, an updated HRA framework was recommended, emphasising the enhancement of the fitness for purpose of HRA, consolidation of the praxis of HRA and improvement of its potential of informed decision-making.

In collaboration with the Slovenian National Building and Civil Engineering Institute (ZAG), we investigated environmental impacts and immobilization mechanisms of cadmium, lead and zinc in geotechnical composites made from contaminated soil and paper ash.

Environmental monitoring

In collaboration with the Environmental Agency from Croatia, we continued with the monitoring of organotin compounds in sea and surface waters.

In the framework of water treatment and environment, we investigated two treatments alternative to the conventional wastewater (WW) treatment, i.e., algal biomass and photochemical treatment. In the case of algal treatment, an alternative treatment that could contribute to the circular economy by valorising reclaimed water and algal biomass, we investigated the fate of selected contaminants of emerging concern (CEC) in lab-scale bioreactors and pilot-scale high-rate algal ponds. The results of these nature-based solutions are encouraging regarding the CEC removal, but we need further research to understand the risks and requirements of safe wastewater and biomass reuse. On the other hand, the developed photocatalytic reactor effectively removed organic dye and bisphenols from the aqueous medium using a combination of adsorption and photocatalysis. Since the photocatalyst deposition method and the reactor are scalable, the removal rates could be further improved.

We continued with the monitoring of the isotope composition of precipitation in Slovenia in the frame of the Slovenian Network of Isotopes in Precipitation (SLONIP) and updated the website https://slonip.ijs.si/.

The monitoring of natural radionuclides within the influential area of the former uranium mine and mill at Žirovski vrh was performed. We also participated in the off-site monitoring of the Krško Nuclear Power Plant (NPP), determining strontium and tritium in environmental samples, as well as tritium and radiocarbon in the gas effluents from the NPP. With the analyses of strontium and tritium, we also participated in the monitoring of radioactivity of drinking water in Slovenia, as well as in the monitoring of the living environment in Slovenia. The methods used for the determination of strontium, tritium and radiocarbon for the monitoring purposes were accredited by the Slovenian Accreditation Board (SA LP-090).

Citizen science and other participatory approaches in the environmental health monitoring

Within the EU Horizon 2020 project CitieS-Health (citieshealth.eu), based on the so-called co-created Citizen Science (CS) approach, aiming at putting citizens' concerns at the heart of the research agenda on environmental epidemiology, 50 citizens were engaged in a study on how the quality of living environment (with the emphasis on noise) and living habits affect the (mental) health and well-being of individuals. In the course of the project, over 350 children also participated in tailored group events organized (e.g., outdoor education and technical days) and four school research assignments were conducted.

URBANOME, a new EU Horizon 2020 project (urbanome.eu) was launched, aimed at promoting urban health, wellbeing and liveability, through systematically integrating health concerns in urban policies and the activities of urban citizens. To this end, within the Ljubljana pilot, intervention is being designed, dealing with the assessment of exposure of individuals to urban stressors using alternative cycling routes.

Education

Within the EU H2020 project A-CINCH and in collaboration with the JSI Centre for Knowledge Transfer in Information Technology, we expanded the production of educational videos for presenting the basics of analytical radiochemistry including analysis of radionuclides in fish and sediment samples.

Infrastructural Centre for Mass Spectrometry (CMS)

The CMS is organized within the Department of Environmental Sciences and connects various mass spectrometers, with which we support research and chemical analysis in research programs and projects in the fields of environmental pollutants, food and feed control and authenticity, the effects of various substances and chemicals on health, etc. The CMS operation is carried out in research areas including analytical chemistry, biochemistry, pharmaceutical and synthetic chemistry, health, food and environment, chemical specifications of elements, quantitative determination of nanoparticle size distribution, spatial distribution of trace elements, determination of bioavailability of essential elements, toxicity products, study of geochemical cycles, identification and structure of biological molecules, active substances and chemotherapeutics in various biological materials, including blood serum, non-target undefined organic compounds and metabolites, quality control and origin of food based on isotope measurements and monitoring transport and source of pollutants in environmental samples and surveillance measurements that will contribute to the protection of human health and air. In collaboration with the other infrastructural centres in the field of structures and properties of substances, the CMS determines qualitative and quantitative analyses of macro components and elements or micro components of trace elements or compounds in complex composite materials and in various matrices: drinking, surface or waste water, waste, foods, medicines, tissues and biological fluids, air, soils, sediments and similar. For this purpose, 12 different mass spectrometers, mostly coupled with chromatographic instruments, are available for research and analysis within the CMS.

Despite the limited scope of work last year due to Covid-19, a lot of quality research, application and development work was carried out in cooperation with industrial and European partners. The results of these measurements are presented in the reports of individual groups of the Department of Environmental Sciences.

Ecological Laboratory with a Mobile Unit

The Mobile Chemical Laboratory of the Ecological Laboratory with a Mobile Unit (ELME) also operates within the Department of Environmental Sciences. The mobile laboratory intervenes within the Civil Protection and Rescue System of Slovenia in the event of environmental pollution and ecological accidents with hazardous substances. In 2021 the ELME Chemical Mobile Laboratory Unit intervened thirteen times in the field as the health of the population was endangered due to hazardous substances, especially polluted air during fires at workplaces or residential areas, spills of hazardous substances into water streams, indirectly endangered drinking water sources and, last year especially, due to an illegal sludge deposition in the natural environment. In addition to emergency interventions, members of the ELME Mobile Chemical Laboratory Unit test their skills at regular ELME drills, receive additional training in using new equipment and improve the knowledge, procedures and analytical methods of the Mobile Ecological Laboratory. Last year, we supplemented the analytical equipment of the mobile chemical laboratory with an X-pid 9500 portable gas chromatograph and an X-act 7000 gaseous and volatile chemical detector of hazardous substances in the air.

Figure 9: Mobile Chemical Laboratory of the Ecological Laboratory with a Mobile Unit (ELME) within the Civil Protection and Rescue System intervenes in the event of environmental pollution and ecological accidents with hazardous substances

Some outstanding achievements in the past year

1. Coordination of the new MSCA ITN FoodTraNet project
2. Within the Comprehensive Analytical Chemistry series, volume 93, Elsevier published the book Analysis and Characterization of Metal-Based Nanomaterials, edited by Radmila Milačič, Janez Ščančar, Heidi Goenaga-Infante and Janja Vidmar.
3. Award for a most outstanding achievement for "Modern organic pollutants - how can we manage them with algae?" This was one of the most excellent research achievements of the University of Ljubljana in 2021 (D. Škufca and E. Heath).
4. European Public Sector Award for the European project APPLAUSE. The EPSA is given by the European Institute of Public Administration (EIPA), promoting the efforts of organizations that develop an innovative, digital and green public sector. "Transformation of invasive alien plants into useful products and raw materials for industry" won the 3rd place in the category Green Public Sector (A. Lapanje and T. Rijavec).
5. Helena Plešnik's master's thesis entitled "Determination of degradation products of bacterial lignin by liquid chromatography combined with mass spectrometry" was part of the Applause project.
6. Johanna Robinson, a young researcher, received an award for the best presentation of a case study entitled "When technology fails: a case study of premature CS tool" at Citizen Science with Application to Nuclear, Seismic and Air Quality Monitoring: APPLICATIONS and Air Quality Monitoring organized by the Abdus Salam International Center for Theoretical Physics (ICTP), 15–19 March 2021.

Some outstanding publications in the past year

1. Castiglioni, Sara Michela, Heath, Ester, et al. New psychoactive substances in several European populations assessed by wastewater-based epidemiology. *Water Research*. 1 May 2021, 195, 1–9. doi: 10.1016/j.watres.2021.116983.
2. Deev, D., Rybkin, Iaroslav, Rijavec, Tomaž, Lapanje, Aleš. When beneficial biofilms on materials is needed: electrostatic attachment of living bacterial cells induces biofilm formation. *Frontiers in Materials*. 2021, 8, 1-624631-14-624631. doi: 10.3389/fmats.2021.624631.
3. Dovjak M., Virant B., Krainer A., Šijanec Zavrl M., Vaupotič J. Determination of optimal ventilation rates in educational environment in terms of radon dosimetry, *International Journal of Hygiene and Environmental Health*. 2021, 234, 113742.
4. Hamzić Gregorčič, S., Ogrinc, N., Frew, R., Nečemer, M., Strojnik, L., Zuliani, T. The provenance of Slovenian milk using $^{87}Sr/^{86}Sr$ isotope ratios. *Foods*. 2021, 10, 8, 1729-1-1729-15. doi: 10.3390/foods10081729.
5. Kovačič, Ana, Gys, Celine, Gulin, Martin Rafael, Gornik, Tjaša, Kosjek, Tina, Heath, David John, Covaci, Adrian, Heath, Ester. Kinetics and biotransformation products of bisphenol F and S during aerobic degradation with activated sludge. *Journal of Hazardous Materials*. 2021, 124079-1-124079-10. ISSN 0304-3894. doi: 10.1016/j.jhazmat.2020.124079.
6. Marković, Stefan, Uršič Valentinuzzi, Katja, Čemažar, Maja, Serša, Gregor, Starešinič, Barbara, Milačič, Radmila, Ščančar, Janez. High spatial resolution imaging of cisplatin and Texas Red cisplatin in tumour spheroids using laser ablation isotope dilution inductively coupled plasma mass spectrometry and confocal fluorescence microscopy. *Analytica Chimica Acta*. 2021, 1162, 338424-1-338424-12. doi: 10.1016/j.aca.2021.338424.
7. Masten, Jasmina, Cillero-Pastor, Berta, Mohren, Ronny, Poklar Ulrih, Nataša, Ogrinc, Nives, Jamnik, Polona. Insight into the antioxidant effect of fermented and non-fermented Spirulina water and ethanol extracts at the proteome level using a yeast cell model. *Antioxidants*. 2021, 10, 9, 1366-1-1366-15. doi: 10.3390/antiox10091366.
8. Roelinger, Alizee, Kocman, David, Robinson, Johanna A., et al. Narrative review of citizen science in environmental epidemiology: setting the stage for co-created research projects in environmental epidemiology. *Environment International*. 2021, 152, 106470-1-106470-13. doi: 10.1016/j.envint.2021.106470.
9. Rovan, Leja, Zuliani, Tea, Horvat, Barbara, Kanduč, Tjaša, Vreča, Polona, Jamil, Qasim, Čermelj, Branko, Bura-Nakić, Elvira, Cukrov, Neven, Štrok, Marko, Lojen, Sonja. Uranium isotopes as a possible tracer of terrestrial authigenic carbonate. *Science of the Total Environment*. 2021, 797, 149103-1-149103-12, doi: 10.1016/j.scitotenv.2021.149103.
10. Runkel, Agneta Annika, Mazej, Darja, Snoj Tratnik, Janja, Tkalec, Žiga, Kosjek, Tina, Horvat, Milena. Exposure of men and lactating women to environmental phenols, phthalates, and DINCH. *Chemosphere*. 2021, 286, part 3, 131858-1-131858-13. doi: 10.1016/j.chemosphere.2021.131858.
11. Schymura, Stefan, Drev, Sandra, Podlipec, Rok, Rijavec, Tomaž, Lapanje, Aleš, Štrok, Marko, et al. Dissolution-based uptake of CeO2 nanoparticles by freshwater shrimp : a dual-radiolabelling study of the

fate of anthropogenic cerium in water organisms. *Environmental Science. Nano*. ISSN 2051-8161. doi: 10.1039/d1en00264c.

12. Strojnik, L., Hladnik, J., Cvelbar Weber, N., Koron, D., Stopar, M., Zlatić, E., Kokalj, D., Strojnik, M., Ogrinc, N. Construction of IsoVoc database for the authentication of natural flavours. *Foods*. 2021, 10, 7, 1550-1-1550-18. doi: 10.3390/foods10071550.

13. Tkalec, Žiga, Kosjek, Tina, Snoj Tratnik, Janja, Stajnko, Anja, Runkel, Agneta Annika, Sykiotou, Marianthi, Mazej, Darja, Horvat, Milena. Exposure of Slovenian children and adolescents to bisphenols, parabens and triclosan: Unirary levels, exposure patterns, determinants of exposure and susceptibility. *Environment International*. 2021, 146, 106172-1-106172-11. doi: 10.1016/j.envint.2020.106172.

14. Verdel, Nada, Rijavec, Tomaž, Rybkin, Iaroslav, Erzin, Anja, Velišček, Žiga, Pintar, Albin, Lapanje, Aleš. Isolation, identification, and selection of bacteria with proof-of-concept for bioaugmentation of white-water from wood-free paper mills. *Frontiers in Microbiology*. 2021, 12, 758702, 1–15. doi: 10.3389/fmicb.2021.758702.

Awards and Appointments

1. Ester Heath and David Škufca: Recognition for the best research achievement of the University of Ljubljana in 2021. University of Ljubljana, Ljubljana, Slovenia. Modern organic pollutants - how can we control them with algae?

2. Žiga Tkalec: Award for the best poster at the Jožef Stefan International Postgraduate School Conference and KMBO Conference, Ljubljana, Jožef Stefan International Postgraduate School. Unexpected exposure of children: novel non-targeted screening workflow

3. Helena Plešnik: Krka's recognition for a master's thesis. Novo mesto, Krka d. d. Determination of bacterial lignin degradation products by liquid chromatography coupled to mass spectrometry

4. Tina Kosjek: Excellent Reviewer Award 2021, Journal of Hazardous Materials, Elsevier

Organization of conferences, congresses and meetings

1. GMOS Train Project meeting, Reactor Centre JSI, Ljubljana, 6–10 October 2021

2. Organization of the student conference of the Jožef Stefan International Postgraduate School and the 15th day of young researchers, 27–28 May 2021 (virtual)

3. Organization of the first hybrid meeting within the COST Action project 'WATer isotopeS in the critical zONe' (WATSON), Faculty of Natural Sciences and Engineering, Ljubljana, 28–29 September 2021

4. Organization of the professional meeting of the Slovenian Association of Geodesy and Geophysics "Research in the field of geodesy and geophysics - 2020", Ljubljana, 28 January 2021 (virtual)

INTERNATIONAL PROJECTS

1. Multielemental Analysis of Moss Samples
   Asst. Prof. Marko Štrok
   Fub AG - Forschungsstelle Fuer

2. EMPIR - EDC-WFD; Metrology for Monitoring Endocrine Disrupting Compounds Under the Water Framework Directive
   Prof. Ester Heath
   Euramet E.v.

3. LIFE18 ENV/SI; LIFE HIDAQUA
   Prof. Radmila Milačič
   European Commission

4. EMPIR; STELLAR; Stable Isotope Metrology to enable Climate Action and Regulation
   Prof. Nives Ogrinc
   Euramet E.v.

5. EMPIR; Si-Hg; Metrology for Traceable Protocols for Elemental and Oxidised Mercury Concentrations
   Prof. Milena Horvat
   Euramet E.v.

6. EMPIR - Food-MetNet; Support for a European Metrology Network on Food Safety
   Prof. Nives Ogrinc
   Euramet E.v.

7. EMPIR - MetroCycleEU; Metrology for the Recycling of Technology Critical Elements to support Europe's Circular Economy Agenda
   Prof. Radojko Jaćimović
   Euramet E.v.

8. Enhancing Nuclear Analytical Techniques to Meet the Needs of Forensic Sciences;

Forensics with Nuclear Methods: Art and Food Forgery, Drugs in Hair
   Prof. Radojko Jaćimović
   IAEA - International Atomic Energy Agency

9. EMPIR - MercOx; Metrology for Oxidised Mercury
   Prof. Milena Horvat
   Euramet E.v.

10. Use of Isotope Techniques for the Evaluation of Water Sources for Domestic Supply in Urban Areas; Multi-isotope characterization of water resources for domestic supply in Ljubljana, Slovenia
    Dr. Polona Vreča
    IAEA - International Atomic Energy Agency

11. Authenticity of High-Quality Slovenian Food Products Using Advanced Analytical Techniques; Implementation of Nuclear Techniques for Authentication of Foods with High-Value Labelling Claims (INTACT Food) (D52042)
    Prof. Nives Ogrinc
    IAEA - International Atomic Energy Agency

12. Isotope Variability of Rain for Assessing Climate Change Impacts; Trends in Isotopic Composition of Precipitation in Slovenia under Climate Change
    Prof. Sonja Lojen
    IAEA - International Atomic Energy Agency

13. TC Regional Project RER/7/014: Improving Environmental Monitoring and Assessment for Radiation Protection in the Region
    Asst. Prof. Marko Štrok
    IAEA - International Atomic Energy Agency

14. COST CA19120 - WATSON; WATer isotopeS in the critical zONe: from groundwater recharge to plant transpiration
    Dr. Polona Vreča
    Cost Association Aisbl

15. COST CA19123 - PHOENIX; Protection, Resilience, Rehabilitation of Damaged Environment
Asst. Prof. Aleš Lapanje
Cost Association Aisbl

16. Measurements and Reporting on Certified Reference Materials BCR-462, BCR-646, ERM-CE477
Asst. Prof. Tea Zuliani
European Commission

17. Stability Testing BCR-679, ERM-CD281 in ERM-CE278k
Asst. Prof. Tea Zuliani
European Commission

18. Training Fees for Hosting Ms. Nurgul Nursapino, Kazakhstan, 04.07.2021 - 30.09.2021, ICTP/IAEA STEP Programme
Asst. Prof. Marko Štrok
Ictp - Centro Internazionale Di Fisica Teorica

19. Training Fees for Fellow Mr. Kylychbek Apiev, 30.08.2021 - 27.11.2021
Prof. Ljudmila Benedik
Ictp - Centro Internazionale Di Fisica Teorica

20. H2020 - ERA-PLANET; The European Network for Observing Our Changing Planet
Prof. Milena Horvat
European Commission

21. H2020 - HBM4EU; European Human Biomonitoring Initiative
Prof. Milena Horvat
European Commission

22. H2020 - NEUROSOME; Exploring the Neurological Exposome
Prof. Milena Horvat
European Commission

23. H2020 - CitieS-Health; Citizen Science for Urban Environment and Health
Dr. David Kocman

24. European Commission

25. H2020 - HERA; Integrating Environment and Health Research: A Vision for the EU
Prof. Milena Horvat
European Commission

26. H2020 - GREENER; InteGRated systems for Effective ENvironmEntal Remediation
Asst. Prof. Aleš Lapanje
European Commission

27. H2020 - EURAD; European Joint Programme on Radioactive Waste Management
Prof. Milena Horvat
European Commission

28. H2020 - FNS-Cloud; Food Nutrition Security Cloud
Prof. Nives Ogrinc
European Commission

29. H2020 - METROFOOD-PP; METROFOOD-RI Preparatory Phase Project
Prof. Nives Ogrinc
European Commission

30. H2020 - A-CINCH; Augmented Cooperation in Education and Training in Nuclear and Radiochemistry
Asst. Prof. Marko Štrok
European Commission

31. H2020 - TUNTWIN; TWINING Towards Advanced Analytical Strategies for Capacity Building and Innovation for the Tunisian Economy: Application to Three Industrial Key Sectors in Tunisia
Prof. Nives Ogrinc
European Commission

32. H2020 - MERFISH; Health-Benefit Understanding of Mercury-Selenium Interactions from Fish to Human
Prof. Milena Horvat
European Commission

33. H2020 - URBANOME; Urban Observatory for Multi-participatory Enhancement of Health and Wellbeing
Prof. Milena Horvat
European Commission

34. H2020 - GMOS-Train; Global Mercury Observation and Training Network in Support to the Minamata Convention
Prof. Milena Horvat
European Commission

35. H2020 - SurfBio; Innovation Hub for Surface and Colloid Biology Research
Asst. Prof. Aleš Lapanje
European Commission

36. H2020 - FoodTraNet; Advanced Research and Training Network in Food Quality, Safety and Security
Prof. Nives Ogrinc
European Commission

37. H2020 - STROMASS; Rapid 90Sr Determination Using Laser Ablation ICP-QQQ-MS
Asst. Prof. Marko Štrok
European Commission

38. Photochemical Fate and Treatment of Pharmaceutical Contaminants in Drinking Water
Asst. Prof. Tina Kosjek
Slovenian Research Agency

39. Mass Balance of Mercury in the Mediterranean Sea
Prof. Milena Horvat
Slovenian Research Agency

40. New Analytical Reference Materials and Techniques for Stable Isotope-Ratio Measurements
Prof. Nives Ogrinc
Slovenian Research Agency

41. Spatial Distribution of d2H, d18O and 87Sr/86Sr in Tap Water and Groundwater from Slovenia
Asst. Prof. Tea Zuliani
Slovenian Research Agency

42. Non-Traditional Isotopes as Novel Tools for Elucidation of Terrestrial Sinks of CO2
Prof. Sonja Lojen
Slovenian Research Agency

43. OrgPlant - Authentication of Organically Grown Plant Products by Novel Stable Isotope Approaches
Prof. Nives Ogrinc
Slovenian Research Agency

RESEARCH PROGRAMMES

1. Modelling and environmental impact assessment of processes and energy technologies
Prof. Borut Smodiš

2. Cycling of substances in the environment, mass balances, modelling of environmental processes and risk assessment
Prof. Milena Horvat

R&D GRANTS AND CONTRACTS

1. Redefinition and revival of copper-free Sonogashira cross-coupling reaction
Prof. Ester Heath

2. Non-traditional isotopes as identifiers of authigenic carbonates
Prof. Sonja Lojen

3. Nanomedicines with antibiotics and probiotics for local treatment of periodontal disease
Asst. Prof. Aleš Lapanje

4. Clinico-pharmacological approach to optimize the therapeutic bleomycin concentration in patients undergoing electrochemotherapy
Asst. Prof. Tina Kosjek

5. Ionom of crop plants for safe and quality food production
Prof. Nives Ogrinc

6. Record of environmental change and human impact in Holocene sediments, Gulf in Trieste
Prof. Sonja Lojen

7. Novel innovative solutions for diaper rash treatment using diapers with probiotic bacteria
Asst. Prof. Aleš Lapanje

8. Methodology approaches in genome-based deversity and ecological plasticity study of truffles from their natural distribution
Prof. Nives Ogrinc

9. Lactic acid fermentation for enrichment of microalgae biomass with new nutrients
Prof. Nives Ogrinc

10. Molybdenum geobiochemical Cycle in modern environments
Prof. Sonja Lojen

11. Impact of endocrine disruptors (bisphenols, parabens, triclosan) and potentially toxic and essential chemical elements on childbirth, infertility and ovarian cancer in Slovenia
Prof. Milena Horvat

12. Monitoring of the clinical and immune response to improve the outcome of combined electrochemotherapy and IL-12 gene therapy in dogs with spontaneous peripheral tumours
Asst. Prof. Tina Kosjek

13. Indentifying the genetic determinants of chemical toxicity in the green alga Chlamydomonas reinhardtii
Prof. Milena Horvat

14. CRIME – CRemation or Inhumation of ancientpopulations? A Multidisciplinary question at the European level
Dr. Doris Potočnik

15. The unrevegled information on soil biodiversity in leached waters
Prof. Nives Ogrinc

16. Subglacial carbonate deposits - a new source for studying the presence of glaciers in a glaciokarstic environment
Prof. Sonja Lojen

17. Neuropsychological dysfunctions caused by low level exposure to selected environmental pollutants in susceptible population – NEURODYS
Prof. Milena Horvat

18. BE MERMAiD - Bioavailable mercury methylation in the Adriatic sea
Prof. Milena Horvat

19. STRAP - Sources, TRansport and fate of persistent Air Pollutants in the environment of Slovenia
Prof. Nives Ogrinc

20. Novel approaches for the estimation of the use of psychoactive pharmaceuticals and illicit drugs by wastewater analysis
Prof. Ester Heath
21. Novel proxies of the Holocene climate variability in stalagmites in Slovenia
Prof. Sonja Lojen
22. Cost-efficient separation of tritium from water with bio-based systems – BIOTRISEP
Asst. Prof. Marko Štrok
23. Innovative isotopic techniques for identification of sources and biogeochemical cycling of mercury in contaminated sites – IsoCont
Prof. Milena Horvat
24. Quality, Safety and Authenticity of INsect PROtein-Based Food and Feed Products
Dr. David John Heath
25. Influence of geotechnical fills from recycled materials on groundwater
Prof. Radmila Milačič
26. EcoFAR: Food security and climate change mitigation by means of ecological farming development - conservation tillage, bioeffectors and sustainable weed management
Prof. Nives Ogrinc
27. Photocatalytic water treatment - development of immobilized catalysts and compact reactor systems
Prof. Ester Heath
28. Illict drugs, alcohol and tobacco: wastewater based epidemiology, treatment efficiency and vulnerability assessment of water catchments
Asst. Prof. Tina Kosjek
29. Identification of Pb sources in the upper Mežiška valley based on Pb isotope composition
Asst. Prof. Tea Zuliani
30. Innovative ECO plasma seed treatment (for sowing and for human and animal diet/ nutrition
Prof. Nives Ogrinc
Ministry of Education, Science and Sport
31. RI-SI EPOS: Development of research Infrastructure for the international competitiveness of Slovenian RRI space-RI-SI
Prof. Janja Vaupotič
Ministry of Education, Science and Sport
32. Circular 4.0: Digital technologies as enabler to foster the transition to the circular economy bythe SME in the Alpine Space area
Asst. Prof. Davor Kontić
Government Office of the Land of Salzburg
33. Danube Hazard m3: Tackling hazardous substances pollution in Danube River Basin by Measuring, Modelling-based Mangement and Capacity building
Prof. Radmila Milačič
Ministry of Finance
34. Cofinancing of LIFE18 ENV/SI; LIFE HIDAQUA: Sustainable Water Management in High Water Demanding Industries
Prof. Radmila Milačič
Ministry of the Environment and Spatial Planning
35. Ecology laboratory with mobile unit
Dr. Dušan Žigon
Ministry of Defence
36. Analyses of tributyl and dibutyltin compounds in water and biota in 2020
Asst. Prof. Tea Zuliani
Ministry of the Environment and Spatial Planning
37. Monitoring of radioactivity in drinking water for years 2020 and 2021 (lot 2)
Asst. Prof. Marko Štrok
Ministry of Health
38. Analysis of honey
Prof. Nives Ogrinc
Slovenian Beekeepers' Association
39. Identification of Pb sources in the upper Mežiška valley based on Pb isotope composition
Asst. Prof. Tea Zuliani
Ministry of the Environment and Spatial Planning
40. Identification of Pb sources in the upper Mežiška valley based on Pb isotope composition
Asst. Prof. Tea Zuliani
Ministry of Health

41. Services; Determination of the Isotopic Composition of Carbon in Sugar Samples
Prof. Nives Ogrinc
42. Different Analyses
Prof. Sonja Lojen
43. Small Services
Dr. Tjaša Kanduč
44. Small Services in the Year 2021
Prof. Milena Horvat
45. Analyses of Metals, TBT and DBT in Sediments, Mussels and Fish
Prof. Janez Ščančar
46. HGKYR - Measurements of Elements in Environmental and Biological Samples from Kyrgyzstan
Prof. Milena Horvat
Médecins Sans Frontieres
47. CROSSING - Crossing Borders and Scales - An Interdisciplinary Approach
Asst. Prof. Aleš Lapanje
Helmholtz-Zentrum Dresden-Rossendorf E.v.
48. Monitoring of the Environmental Fingerprint in Graviera Naxou PDO Product for Certification of Authenticity and Geographical Origin - Sr Isotopes and H, O, C, N Stable Isotopes
Asst. Prof. Tea Zuliani
Agricultural Cooperatives Union
49. Dual (Oxygen and Strontium) Stable Isotope-Based Wood Provenancing
Asst. Prof. Tea Zuliani
Stefan Cel Mare University of Suceava
50. Radon Mapping and Radon Risk Assessment in Georgia
Prof. Janja Vaupotič
Ivane Javakhishvili Tbilisi State University
51. Influence of Application of Mineral Fertilizers on Accumulation Ability of Radionuclides and Heavy Metals in Root Vegetables
Asst. Prof. Marko Štrok
Al-farabi Kazakh National University
52. Development of Training/Education Modules on Human Monitoring
Prof. Milena Horvat
World Health Organization

NEW CONTRACTS

1. Measurements of gaseous effluents, specific analysis of H-3 and C-14 in year 2021
Asst. Prof. Marko Štrok
Krško Nuclear Power Plant
2. illicit drugs, alcohol and tobacco: wastewater based epidemiology, treatment efficiency and vulnerability assessment of water catchments
Asst. Prof. Tina Kosjek
Mariborski Vodovod d. d.
3. illicit drugs, alcohol and tobacco: wastewater based epidemiology, treatment efficiency and vulnerability assessment of water catchments
Asst. Prof. Tina Kosjek
JP CČN Domžale-kamnik d. o. o.
4. illicit drugs, alcohol and tobacco: wastewater based epidemiology, treatment efficiency and vulnerability assessment of water catchments
Asst. Prof. Tina Kosjek
JP Vodovod-kanalizacija D.o.o
5. Environmental radioactivity monitoring in the vicinity of the Krško Nuclear Power Plant (drinking water, air, food, Sava River, precipitation, soil and external radiation in the environment with the dose assessment)
Asst. Prof. Marko Štrok
Krško Nuclear Power Plant
6. Environmental radioactivity monitoring in the vicinity of the Krško Nuclear Power Plant in connection with Hydro Power Plant Brežice for the years 2020 and 2021
Asst. Prof. Marko Štrok
Krško Nuclear Power Plant

VISITORS FROM ABROAD

1. Klaudia Block-Laszewska, University of Gdańsk, Gdańsk, Poland, 10 June–31 August 2021
2. prof. dr. Alexander Osmolovskiy, Lomonosov Moscow State University, Moscow, Russia, 11–13 June 2021
3. prof. dr. Alexander Gusev, Derzhavin Tambov State University, Tambov, Russia, 30 June–7 July 2021
4. Nurgul Nursapina, Al-Farabi Kazakh National University, Almaty, Kazakhstan, 4 July–30 September 2021

5. dr. Elvira Bura Nakić, Institut Ruđer Bošković, Zagreb, Croatia, 22 August–4 September 2021
6. dr. Tamara Marković, Hrvatski geološki institut, Zagreb, Croatia, 1–8 September 2021
7. Igor Karlović, Hrvatski geološki institut, Zagreb, Croatia, 1–8 September 2021
8. Kylychbek Apiev, Agency for Tailings Management, Ministry of Emergency Situations of the Kyrgyz Republic, Bishkek, Kirgizstan, 1 September–27 November 2021
9. dr. Daniele Penna, University of Florence, Firenze, Italy, 30 September 2021
10. dr. Ilja van Meerveld, University of Zürich, Switzerland, 30 September 2021

11. dr. Jana von Freyberg, École polytechnique fédérale de Lausanne, Switzerland, 30 September 2021
12. dr. Francesca Scandellari, U-Series srl, Bologna, Italy, 30 September 2021
13. Giulia Zuecco, University of Padova, Italy, 30 September 2021
14. dr. Petra Žvab Rožič, University of Ljubljana, 30 September 2021
15. dr. Aurelien Dommergue, UGA, Grenoble, France, 6–7 October 2021
16. dr. Lars Eric Heimbürger-Boavida, Mediterranean Institute of Oceanography, Marseille, France, 6–10 October 2021
17. dr. David Amouroux, UPPA, Pau Cedex, France, 6–10 October 2021
18. dr. Joel Knoery, Ifremer, Nantes, France, 6–10 October 2021
19. dr. Sofi Jonsson, Stockholm University, Stockholm, Sweden, 6–10 October 2021
20. dr. Ralph Ebinghaus, Helmholtz-Zentrum Hereon, Geesthacht, Germany, 6–10 October 2021
21. dr. Ian Hedgecock, Institute of Atmospheric Pollution Research of the Italian National Research Council, Monterotondo, Italy, 6–10 October 2021
22. dr. Jeoren Sonke, CNRS, Paris, France, 6–10 October 2021
23. dr. Volker Matthias, Helmholtz-Zentrum Hereon, Geesthacht, Germany, 6–10 October 2021
24. dr. Johannes Bieser, Helmholtz-Zentrum Hereon, Geesthacht, Germany, 6–10 October 2021
25. dr. Andreja Gutmaher, IOS, Maribor, 6–10 October 2021
26. dr. Aljoša Košak, IOS, Maribor, 6–10 October 2021
27. Alquin Maximillian Koenig, UGA, Grenoble, France, 6–10 October 2021
28. Alina Kleindienst, UPPA, Pau, France, 6–10 October 2021
29. Isabel García Arévalo, Ifremer, Nantes, France, 6–10 October 2021
30. Sonja Gindorf, Stockholm University, Stockholm, Sweden, 6–10 October 2021
31. Charlotte Haugk, Stockholm University, Stockholm, Sweden, 6–10 October 2021
32. Prasad Shelke, CNR-IIA, Rome, Italy, 6–10 October 2021
33. David Amptmeijer, Helmholtz-Zentrum Hereon, Geesthacht, Germany, 6–10 October 2021
34. Koketso Michelle Molepo, Helmholtz-Zentrum Hereon, Geesthacht, Germany, 6–10 October 2021
35. Charikleia Gournia, CNR-IIA, Rome, Italy, 6–10 October 2021
36. Allwin Mabes Raj, IOS, Maribor, 6–10 October 2021 and 5 November–31 December 2021

STAFF

Researchers
1. Prof. Ljudmila Benedik
2. Raghuraj Singh Chouhan, B. Sc.
3. Asst. Prof. Ingrid Falnoga
4. Dr. David John Heath
5. Prof. Ester Heath
6. **Prof. Milena Horvat, Head**
7. Prof. Radojko Jaćimović
8. Dr. Tjaša Kanduč
9. Dr. Norbert Kavasi
10. Dr. David Kocman
11. Asst. Prof. Davor Kontić
12. Asst. Prof. Tina Kosjek
13. Asst. Prof. Jože Kotnik
14. Asst. Prof. Aleš Lapanje
15. Prof. Sonja Lojen
16. Dr. Darja Mazej
17. Prof. Radmila Milačič
18. Prof. Nives Ogrinc
19. Asst. Prof. Tomaž Rijavec
20. Prof. Borut Smodiš
21. Prof. Janez Ščančar
22. Asst. Prof. Zdenka Šlejkovec
23. Asst. Prof. Marko Štrok
24. Prof. Janja Vaupotič
25. Dr. Janja Vidmar
26. Dr. Polona Vreča
27. Asst. Prof. Tea Zuliani
28. Dr. Dušan Žigon

Postdoctoral associates
29. Dr. Ermira Begu
30. Dr. Marta Jagodic Hudobivnik
31. Dr. Ana Kovačič
32. Dr. Bor Krajnc
33. Dr. Doris Potočnik
34. Dr. Leja Rovan
35. Janja Snoj Tratnik, B. Sc.
36. Dr. Anja Stajnko
37. Dr. Igor Živković

Postgraduates
38. Saeed Waqar Ali, M. Sc.
39. Eirini Andreasidou, M. Sc.
40. Teodor-Daniel Andron, M. Sc.
41. Tine Bizjak, M. Sc.
42. Dominik Božič, B. Sc.
43. Jan Gačnik, B. Sc.
44. Tjaša Goltnik, B. Sc.
45. Pia Leban, B. Sc.
46. Katarina Marković, B. Sc.
47. Jasmina Masten Rutar, B. Sc.
48. Klara Nagode, B. Sc.
49. Rok Novak, B. Sc.
50. Neža Palir, B. Sc.
51. Johanna Amalia Robinson, B. Sc.
52. Agneta Annika Runkel, B. Sc.
53. Lidija Strojnik, B. Sc.
54. Žiga Tkalec, B. Sc.
55. Anja Vehar, B. Sc.
56. Sreekanth Vijayakumaran Nair, M. Sc.
57. Maja Zugan, B. Sc.

Technical officers
58. Karolina Trentelj, B. Sc.
59. Vanja Usenik, B. Sc.
60. Tina Vrabec, B. Sc.

Technical and administrative staff
61. Barbara Svetek, B. Sc.
62. *Zdenka Trkov, B. Sc., retired 26.05.21*
63. Stojan Žigon

BIBLIOGRAPHY

ORIGINAL ARTICLE

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THESES AND MENTORING

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DEPARTMENT OF AUTOMATION, BIOCYBERNETICS AND ROBOTICS E-1

The research strategy within our department (http://abr.ijs.si/) supports a variety of multi- and interdisciplinary research projects. Specifically, our research combines the fields of robotics (including robot learning, intelligent control, humanoids, cognitive robotics, and robot vision), industrial robotics and automation, factories of the future, biomechanics, biocybernetics, ergonomics and environmental physiology. The common theme of our research endeavours to date has been optimizing "the behaviour of man and machine", accounting for the interactions with the environment. By combining engineering and life sciences we have been able to make breakthrough contributions in the areas of robot learning based on imitation and deep neural networks, development of a planetary habitat simulation facility, reconfigurable robotic workcells, humanoid robotic systems, exoskeletons, manikins enabling the evaluation of protective garments for industry and recreation, new strategies for physical human-robot interaction, and a medical treatment for frostbite.

The department maintains the programme group Automation, Robotics and Biocybernetics in the field of Production Technologies (led by prof. dr. Igor B. Mekjavic). Members of the department participate in numerous EU projects in the areas of robotics and artificial intelligence, factories of the future, health, and space technologies. In 2021 we coordinated the ReconCycle Horizon 2020 project. We are also active in transferring our research results to various applications through direct collaboration with industry.

Research in humanoid robotics and robot learning is primarily conducted within the Humanoid and Cognitive Robotics Lab (led by dr. Bojan Nemec), which operates within the department. The aim of this laboratory is to create robots that can acquire new knowledge through learning and collaborating with people in their natural environments. Another laboratory that operates within the department is the Laboratory for Neuromechanics and Biorobotics, which is led by prof. dr. Jan Babič. The focus of this lab is to integrate the results of biomechanics, neurophysiology and robotics to study human motor control and develop new robot systems that can effectively assist people with their daily activities.

Head:
Prof. Aleš Ude

By maintaining a critical mass of researchers in the areas of robotics, automation and life sciences within one department, we have managed to foster exciting multidisciplinary projects.

During the past year our research focused on the development of reconfigurable robotic systems for factories of the future, automation of production processes in manufacturing, new robot-learning methodologies primarily based on kinesthetic teaching and deep learning, human-robot collaboration, development of new control methods for robotic assistive devices such as exoskeletons, studies of human physiology in extreme environments, evaluation of protective equipment, as well as the development of biomedical methods.

Robotics

In 2021 we continued coordinating another Horizon 2020 project, called **ReconCycle** (Self-reconfiguration of a robotic workcell for the recycling of electronic waste, http://www.reconcycle.eu/). The main aim of the project is to introduce **self-reconfigurable hardware and software for the disassembly of electronic devices**, based on a reconfigurable robotic cell developed within the ReconCell project, http://www.reconcell.eu/. The challenge of this project is to provide methodologies for a re-design of the recycling cell including the location of robots and other elements in the workcell and the choice of grippers and sensing systems. On the software side, approaches to the fast re-programming and adaptation of manipulation actions for soft robots and grippers suitable for recycling tasks need to be provided. Soft components make grasping and compliant control easier, but they can be problematic with regard to assembly tasks that usually rely on high-precision position control. However, high precision is less important for disassembly where physical constraints can guide compliant robot movements to successfully accomplish the task.

In the H2020 project ReconCycle coordinated by our department we aim at substantially increasing the degree of automation in recycling by introducing new robot-learning technologies.
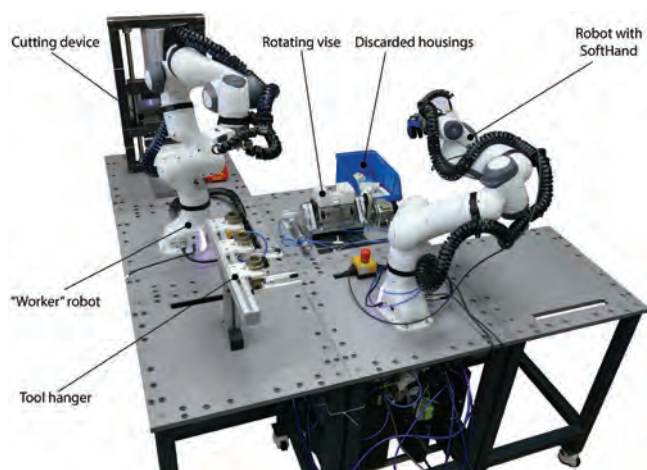
Figure 1: Reconfigurable cell for recycling of electronic devices

Within the AnDy H2020 project, completed in 2021, we worked on endowing robots with the ability to control physical collaboration through intentional interactions.
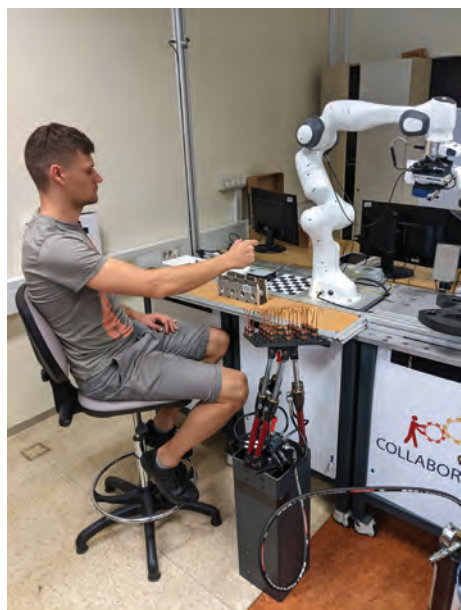
Figure 2: Optimal design of a collaborative robotic cell

In 2021 we finalized the new experimental laboratory Cobotat – Laboratory for Advancing Collaborative Robot Behaviors in Physical Human-Robot Interaction Scenarios.

We also worked on a Horizon 2020 project in the area of collaborative robotics, CoLLaboratE (Enabling genuine human-robot collaboration for performing assembly tasks in a co-production cell, https://collaborate-project.eu). CoLLaboratE aims to **revolutionize the way industrial robots learn to cooperate with human workers** when performing new manufacturing tasks. In 2021 we developed an approach to efficient human-robot task execution using visual information processed by recurrent deep neural networks. We have shown how multimodal visual and force information can be used for collaborative task learning. Another important result was the implementation of a new optimization procedure to design collaborative workspaces, taking into account the capabilities of robots and human workers.

In the area of humanoid robotics we conducted several studies focusing on **humanoid robot sensorimotor skill learning** where we exploit the mobility of a humanoid robot, while taking into account its stability. We demonstrated that programming by demonstration, which is suitable for humanoid robots due to their similarities to humans, can be supplemented by reinforcement learning to improve the newly acquired mobile skills. The advantage of the approach is that it can be used effectively in situations where no accurate models of robot and task dynamics are available.

In the field of exoskeleton robotics we **finalized analyses of parabolic flight experiments** where we investigated the possibilities to **employ exoskeleton devices** to assist astronauts during space missions. We demonstrated that the use of an exoskeleton, compensating for the variance in gravity affecting the human arm movements, mitigates the effects of altered gravity on motor control. In a series of three publications we showed that a robotic exoskeleton had a significant effect on the duration of movements, the accuracy of pointing and muscle activities. Moreover, we established an evidence-based methodology that can be used to train astronauts before their space missions. Specifically, we have shown that motor imagery alone cannot be used to adapt to a novel gravitational environment. On the other hand, a robotic exoskeleton that emulates the gravitational effects of micro gravity and hyper gravity can efficiently contribute to timely motor adaptations.

We also studied the use of wearable technologies in the prevention of acute and chronic injuries of athletes due to motion asymmetries. We developed a portable measuring system that measures the motion of an athlete's body during sport activities, analyses the motion in real time and gives the athlete feedback on how to change the motion to avoid the stress and possible injury. The measuring system was protected with a Slovenian patent application. In 2021 we **successfully completed the AnDy Horizon 2020 project** (https://andy-project.eu), within which we implemented and evaluated different exoskeleton solutions for industrial settings.

We continued our long-standing line of research in the field of physical human-robot collaboration where we developed an innovative control approach that utilizes probabilistic movement primitives in combination with flow controllers to **generate predictions of user movements in real-time**. We employed our method in three scenarios: in exoskeleton-assisted arm reaching, in human collaboration with a robot arm and in predicting foot step locations.

Under the Director's Fund **Cobotat** project (Laboratory for Advancing Collaborative Robot Behaviors in Physical Human-Robot Interaction Scenarios, http://cobotat.ijs.si/), led by dr. Tadej Petrič, we successfully completed the PhRoCiety project (Collaborative Capabilities in Physical Human-Robot Interaction Scenarios, http://cobotat.ijs.si/projects/phrociety-2), which aimed to improve **cognitive understanding and control systems for collaborative physical interactions** between multiple agents, where the agents are either humans or robots. In collaboration with Idiap, we continued the implementation of the SWITCH project (Learning by Switching Roles in Physical Human-Robot Collaboration, https://switch-project.github.io/), co-funded by the SNSF in Switzerland. The main contribution of the SWITCH project in 2021 was the collection of several datasets on forces and motions in different task modalities. Many laboratory studies were conducted to investigate the physical interaction between two people in a standing-up task. Based on these data, we developed models to probabilistically learn the behaviour of the two agents (the assistant and the assisted). We then used these models to develop control systems for humanoid robots with predictive behaviour. We also used the obtained data to develop a new quasi-passive mechanism for a knee exoskeleton. The developed mechanism is patent pending.

The main objective of the **TRINITY** project (https://trinityrobotics.eu/), another Horizon 2020 project at our department, is to create a network of multidisciplinary and synergistic local digital innovation hubs (DIHs) including research centers, companies and university groups, covering a wide range of topics that can contribute to agile production: advanced robotics as the driving force and digital tools, data privacy and cyber-security technologies, supporting the introduction of advanced robotic systems in the production processes. In 2021 we focused on the practical evaluation of demonstrators that showed **the industrial potential of programming by demonstration** for the specification of skilled operations in contact with the environment and of **passive reconfiguration** using a fixturing system built from Stewart platforms. In the future the modules from our demonstrators will be offered to manufacturers.

Figure 3: Quasi-passive knee exoskeleton

Automation and robotics in industrial production processes

In the **QU4LITY** H2020 project (https://qu4lity-project.eu) we aim to demonstrate, in a realistic, measurable and replicable way, an open, certifiable and highly standardised, SME-friendly and transformative shared data-driven ZDM product and service model for Factory 4.0 through 14 pilot lines. We collaborated with the Slovenian company Kolektor and developed a cell at the end of a moulding line for visual quality inspection. The cell enables new robot-supported approaches to visual quality inspection based on deep learning and automated workcell reconfiguration technologies. In 2021 we focused on the experimental evaluation of the developed technologies.

A vital mission of our department is the transfer of our research results to industrial applications. In recent years our department has been working towards the implementation of the **Smart specialization strategy S4**. As part of the Strategic Research and Innovation Partnership of the Factory of the Future (SRIP FoF), we **chaired** the SRIP FoF Board of Directors, **coordinated** the SRIP FoF Horizontal Network (Key Enabling Technology) "Robotics", thus providing support for the introduction of advanced robotic technologies into factories of the future, being developed by the Slovenian industry. In 2021 the SRIP FoF started to implement a new program to foster cooperation of manufacturing companies with the research departments at the universities and institutes and transfer the latest robotics research results into industrial practice.

In collaboration with two leading Slovenian manufacturing companies, Gorenje and Unior, we developed a comprehensive system for quality control in the production processes.

In the scope of the Slovenian Smart Specialization Strategy, we have joined the ROBKONCEL project, whose main goal is to develop **a comprehensive system for quality control in the production process** and inspection of finished products. As part of the project, we developed two demonstration robotic cells for the final quality inspection of ovens at Gorenje and the control of forgings at Unior. The oven-inspection cell for Gorenje is equipped with a collaborative robot Frank Emika Panda, while in the forging control cell for Unior, we used the Universal Robots UR10. We developed an appropriate software environment for programming collaborative robots, which supports modern robot-learning technologies. We also proposed new approaches that improve the flexibility and adaptability to product changes and inspection procedures. The proposed procedures were validated on several samples of products. We evaluated the functionalities that the final cell must provide in the production, especially from the point of view of productivity.

Environmental physiology and ergonomics

Life-science research in our department focuses on the physiology and pathophysiology of humans in extreme environments. We contribute to the development of new strategies and equipment to mitigate the effects of environmental factors on human health and well-being, and enhance the safety and productivity of workers in industrial and military environments.

Gravitational physiology: The Jožef Stefan Institute Planetary Habitat Simulation facility in Planica, maintained by our department, was approved as a European Space Agency (ESA) ground-based facility in 2020. The PlanHab facility is one of 11 such ESA ground-based facilities in Europe where scientists can conduct ESA-funded projects.

As a consequence of this development, members of the E1 team are members of ESA's Advisory Board focusing on future research programmes coordinated by the Human and Robotic Exploration division of ESA. The current programme, in which the E1 team has a significant role, covers the evaluation of countermeasures that would prevent the adaptation of physiological systems to microgravity. Specifically, the focus is on the

Figure 4: Experimental environment to study the effects of local gravity compensation on motor control
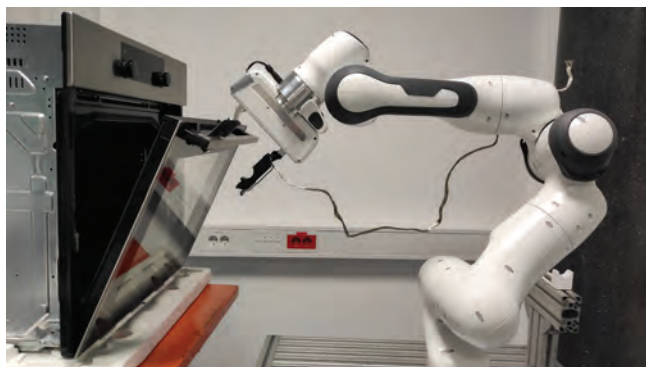
Figure 5: Testing of ovens for quality control

evaluations of the efficacy of resistance vibration exercise in combination with artificial gravity. Since the anticipated environment of future space vehicles and habitats will be hypoxic, the PlanHab facility will coordinate studies investigating the mitigation of muscle atrophy, loss of bone mass and cardiovascular deconditioning, among others, in a hypoxic environment. For this new research endeavour, the European Space Agency **installed a short-arm human centrifuge** (valued at €2 m) at the newly established Gravitational Physiology Laboratory in the PlanHab facility.

Protective clothing: Within the framework of the ReMOS (Regulation of the microenvironment of clothing systems) project supported by the Slovenian Ministry of Defence, we established a consortium of companies with the aim of developing smart clothing for the Slovenian armed forces. As the project coordinator, we lead the activities of industrial partners in the consortium. Our partners cover the complete process of clothing development, from yarn and fabric to the final products, which include embedded sensors and processors to provide regulation of the microenvironment within cooling vests, and alerting to the potential of cold injury.

Our contribution within ReMOS was the development of a software application that would provide support in the preparation for missions in extreme environmental conditions. For this purpose, we evaluated the thermal and evaporative characteristics of all protective clothing combinations available to the Slovenian armed forces. Using these data, together with the soldier's anthropometry and anticipated activity, and the prevailing or anticipated environmental conditions, **the software application provides suggestions for optimal protective clothing ensembles** for the environmental conditions.

On 1 October 2021 we inaugurated the Gravitational Physiology Laboratory at the JSI PlanHab facility in Planica.

Figure 6: Inauguration of the Gravitational Physiology Lab in Planica. From left to right: Josef Aschbacher (director, ESA), Boštjan Zalar (director, JSI), Simona Kustec (Slovenian minister of Education, Science and Sport), Igor Mekjavic (E1), and Adam McDonnell (E1)

Global warming: Summer heatwaves are becoming more frequent, greater in intensity and longer in duration. The HEAT-SHIELD Horizon 2020 project was initiated to assess the effect of heatwaves on the productivity of workers in five major EU industries (manufacturing, construction, transportation, tourism and agriculture), representing 40% of EU's GDP and 50% of its workforce. The aim of the project was to **explore and develop the strategies that would mitigate the heat stress** in these industries and the resultant heat strain on the workers. Successful mitigation strategies will ensure the health of the workforce, and can also shield our economy from the negative effects of climate change.

Within HEAT-SHIELD we collaborated with the Slovenian manufacturing company Odelo. Briefly, the company operates 24/7 and manufactures automobile rear lights. The heat generated by the machinery can only be partly removed by the existing ventilation systems. This becomes an issue during the summer months and especially during heat waves when heat accumulation becomes too severe. Field studies conducted at the plant confirmed that such conditions affect productivity also in the periods following the heat waves, suggesting insufficient recovery of the workers. As a consequence, a longer period of heat exposure may affect work productivity because of a cumulative effect that results from an inability of the workers to recover properly after leaving work. Therefore, it was proposed that the company implements several actions to reduce the problem of productivity loss and improve the well-being of workers.

Individual variability: It is well appreciated that there is a great deal of individual variability in the responses of astronauts to microgravity. This is also evidenced in the magnitude of the loss of muscle and bone mass, and of cardiovascular deconditioning during space analogues such as bed rest and dry immersions. Our department

In 2021 we successfully completed the HEAT-SHIELD H2020 project, within which we investigated how to increase the thermal resilience of workers in the context of global warming.

initiated the Slovene Bed Rest Programme in 2001. Since then numerous such studies have been conducted. Under contract with the European Space Agency, we used these data to explore the possibility of determining the individual variability in the **responses of physiological systems to hypoxic and normoxic bed rest** conducted within the framework of the Slovene Bed Rest Programme. The data obtained with the Planica bed-rest studies were re-analysed to determine the magnitude, significance and physiological relevance of the variability in the physiological responses to normoxic and hypoxic bed rest. The results demonstrated a significant degree of individual variability, particularly in the inactivity / unloading-induced muscle atrophy and in the psychological status of the participants during bed rest.

Core-temperature prediction: The need for rapid and accurate monitoring of deep body temperatures in humans has arisen, in part, as a result of two major global requirements: rising temperature/heatwaves and the COVID-19 pandemic. Indirect measurement of deep-body temperature calculated using algorithms from skin temperature has become increasingly common; however, its validity and accuracy have been questioned. We conducted the simulation of a 3-day heatwave bookended by 3 days of normal conditions, during which continuous measurement of deep-body and skin temperature was conducted. Our results demonstrate that utilising **skin temperature as a predictor of deep-body temperature is physiologically unsuitable** due to a large and inconsistent error.

Haemoglobin mass of athletes participating in aquatic sports: The overall objective of this project is to investigate the level of hypoxia present in aquatic athletes during training and how this may influence their performance. With industrial partners, we are contributing to the development and evaluation of the technology that will not only assist in remotely monitoring athletes in general but, more importantly, provide a tool for healthcare workers dealing with Covid-19 patients. Specifically, we work on the **assessment of the degree of tissue hypoxia experienced during swimming** and examine any long-term hypoxic acclimation, reflected primarily in the haemoglobin mass.

Figure 7: Sweating thermal manikins for testing protective garments

Some outstanding publications in the past year

1. T. Gašpar, I. Kovač, A. Ude (2021) Optimal layout and reconfiguration of a fixturing system constructed from passive Stewart platforms, Journal of Manufacturing Systems, 60:226–238.
2. M. Jamšek, T. Kunavar, U. Bobek, E. Rueckert, J. Babič (2021) Predictive exoskeleton control for arm-motion augmentation based on probabilistic movement primitives combined with a flow controller, IEEE Robotics and Automation Letters, 6(3):4417–4424.
3. J. T. Royal, O. Eiken, M. E. Keramidas, A. Mcdonnell, I. B. Mekjavić (2021) Heterogeneity of hematological response to hypoxia and short-term or medium-term bed rest, Frontiers in Physiology, 12(777611):1–14.
4. B. Nemec, K. Yasuda, A. Ude (2021) A virtual mechanism approach for exploiting functional redundancy in finishing operations, IEEE Transactions on Automation Science and Engineering, 18(4):2048–2060.
5. Z. Lončarević, A. Gams, S. Reberšek, B. Nemec, J. Škrabar, J. Skvarč, A. Ude (2021) Specifying and optimizing robotic motion for visual quality inspection, Robotics and Computer-Integrated Manufacturing, 72(102200):1–14.
6. U. Ciuha, A. Sotiridis, T. Mlinar, J. T. Royal, O. Eiken, I. B. Mekjavić (2021) Heat acclimation enhances the cold-induced vasodilation response, European Journal of Applied Physiology, 121(11):3005–3015.

Organization of conferences, congresses and meetings

1. 20th International Conference on Advanced Robotics (ICAR), Ljubljana, 7–10 December 2021

Awards and Appointments

1. Tilen Brecelj and Tadej Petrič: Best Research Paper Award, Futuroscope-Poitiers, France, RAAD 2021, Angular Dependency of the Zero Moment Point
2. Timotej Gašpar: Vodovnik Award for Doctoral Study, Ljubljana, Faculty of Electrical Engineering, University of Ljubljana, Technologies for fast reconfiguration of adaptive robotic workcells

Organization of conferences, congresses and meetings

1. H2020 ReconCycle meeting, 26 May 2021 (virtual)
2. ICAR 2021 - 20th International Conference on Advanced Robotics, Ljubljana, 7–10 December 2021 (hybrid)

Patents granted

1. Igor Kovač, Cardan joint, EP3615823 (B1), European Patent Office, 02. 06. 2021.
2. Anton Umek, Boris Jerman, Mitja Gliha, Anton Kos, Iztok Špan, Link member for connection of a gripping assembly to a hydraulic crane arm with integrated dynamic weighing assembly, EP3649071 (B1), European Patent Office, 24. 02. 2021.
3. Nejc Šarabon, Monika Pavlović, Andrej Trošt, Jan Babič, Multi-accelerometer system and method for evaluating mechanical stress during walking and running SI25959 (A), Slovenian Intellectual Property Office, 30. 07. 2021.

INTERNATIONAL PROJECTS

1. Manufacture of Finger and Two Hands of the Manikin, and National Instruments Measuring Software
   Prof. Igor Mekjavić
   W. L. Gore & Associates GmbH
2. ALITO: Testing of Face Masks
   Prof. Igor Mekjavić
   Kimberly-Clark
3. COST CA16116 - 20786; Wearable Robots for Augmentation, Assistance or Substitution of Human Motor Functions
   Prof. Jan Babič
   Cost Office
4. ESA - Individual Variation in Human Response to prolonged Bed Rest in Slovenia Bed Rest Programme
   Prof. Igor Mekjavić
   ESA/Estec.
5. COST CA16116 Summerschool Wearable Robotics 2021
   Prof. Jan Babič
   Cost Association Aisbl
6. H2020 - HEAT-SHIELD; Integrated Inter-Sector Framework to increase the Thermal Resilience of European Workers in the Context of Global Warming
   Prof. Igor Mekjavić
   European Commission
7. H2020 - An.Dy; Advancing Anticipatory Behaviors in Dyadic Human-Robot Collaboration
   Prof. Jan Babič
   European Commission
8. H2020 - CoLLaboratE: Co-production CeLL performing Human-RobotCollaborative AssEmbly
   Prof. Bojan Nemec
   European Commission
9. H2020 - TRINITY; Digital Technologies, Advanced Robotics and increased Cyber-Security for Agile Production in Future European Manufacturing
   Prof. Aleš Ude
   European Commission
10. H2020 - QU4LITY; Digital Reality in Zero Defect Manufacturing
    Prof. Aleš Ude
    European Commission
11. H2020 - COVR: EXOSAFE; A Mechatronic Leg Replica to Benchmark Human-Exoskeleton Interaction
    Prof. Jan Babič
    European Commission
12. H2020 - ReconCycle; Self-reconfiguration of a Robotic Workcell for the Recycling of Electronic Waste
    Prof. Aleš Ude
    European Commission
13. Learning Cross-Task Generalization for Model-Predictive Control: Application to Dynamic Humanoid Behaviors
    Prof. Andrej Gams
    Slovenian Research Agency
14. The Interaction of Regional Thermal and Baroreflex Regulation of the Peripheral Circulation
    Prof. Igor Mekjavić
    Slovenian Research Agency
15. Generation and Learning of Adaptive Cyclic Movements in Assist-As-Needed Applications for Human-Robot Interaction
    Asst. Prof. Tadej Petrič
    Slovenian Research Agency
16. HE - EUROfusion; WP17: RM_HE-FU
    Prof. Aleš Ude
    European Commission

RESEARCH PROGRAMME

1. Avtomation, robotics and biocybernetics
   Prof. Igor Mekjavić

R&D GRANTS AND CONTRACTS

1. Mechanisms of hypoxia (in)tolerance in prematurely born individuals
   Prof. Tadej Debevec
2. X-ADAPT: Cross-adaptation between heat and hypoxia - novel strategy for performance and work-ability enhancement in various environments
   Prof. Tadej Debevec
3. The effect of hypercapnic exercise on intracranial pressure and the eye
   Prof. Igor Mekjavić
4. Towards Cooperative Robot Behaviors in Physical Human-Robot Interaction Scenarios
   Asst. Prof. Tadej Petrič
5. Learning by Switching Roles in Physical Human-Robot Collaboration (SWITCH)
   Asst. Prof. Tadej Petrič
6. The use of Resistive Vibration Exercise (RVE) to mitigate hypoxic inactivity induced cartilage degeneration: implications for Covid-19 patients
   Dr. Adam Mc Donnell
7. Body asymmetries as a risk factor in musculoskeletal injury development: studying etiological mechanisms and designing corrective interventions for primary and tertiary prevenitve care
   Prof. Jan Babič

VISITORS FROM ABROAD

1. Gregoire Millet, University of Lausanne, Switzerland, 3 May – 30 June 2021
2. Giorgio Manferdelli, University of Lausanne, Switzerland, 3 May – 30 June 2021
3. Justin Lawley, University of Innsbruck, Austria, 12–16 May 2021
4. Sebastian Ruiz, University of Göttingen, Germany, 21 June – 9 July 2021
5. Nikola Knežević, University of Belgrade, Serbia, 10-25 July 2021
6. Branko Lukić, University of Belgrade, Serbia, 10-25 July 2021
7. Kubra Karacan, Technische Universität München, Germany, 29 November – 3 December 2021

STAFF

Researchers
1. Prof. Jan Babič
2. Prof. Tadej Debevec*
3. Prof. Andrej Gams
4. Prof. Polonca Jaki Mekjavić*
5. Asst. Prof. Igor Kovač
6. Prof. Jadran Lenarčič
7. Dr. Adam Mc Donnell
8. Prof. Igor Mekjavić
9. Prof. Bojan Nemec
10. Asst. Prof. Tadej Petrič
11. Dr. Anton Ružić
12. *Prof. Blaž Stres*, left 01.07.21*
13. **Prof. Aleš Ude, Head**
14. Asst. Prof. Leon Žlajpah
Postdoctoral associates
15. Dr. Edwin Johnatan Avila Mireles
16. Dr. Tilen Brecelj
17. Dr. Urša Ciuha
18. *Dr. Jernej Čamernik, on leave since 01.02.21*
19. Dr. Miha Deniša
20. *Dr. Miha Dežman, on leave since 01.05.21*
21. *Dr. Timotej Gašpar*, left 01.04.21*
22. Dr. Rok Pahič*
23. *Dr. Tim Podlogar, left 01.07.21*
24. Dr. Desy Salvadego
Postgraduates
25. Benjamin Fele, B. Sc.
26. Jason Thomas Fisher, M. Sc.
27. Marko Jamšek, B. Sc.
28. Jaka Jereb, B. Sc.
29. Tjaša Kunavar, B. Sc.
30. Boris Kuster, B. Sc.
31. Zvezdan Lončarević, B. Sc.
32. Matija Mavsar, B. Sc.
33. Luka Mišković, M. Sc.
34. Tinkara Mlinar, M. Sc.
35. Benjamin Jonathan Narang, M. Sc.
36. Peter Nimac, B. Sc.
37. Joshua Toby Royal, M. Sc.

38. Mihael Simonič, M. Sc.
39. Riccardo Sorrentino, M. Sc.
Technical officers
40. Mitja Gliha, B. Sc.
41. Rebeka Kropivšek Leskovar, B. Sc.
42. Matevž Majcen Hrovat, B. Sc.
43. Primož Radanovič, B. Sc.
44. Simon Reberšek, B. Sc.
45. *Matej Štefanič, B. Sc., left 01.11.21*

46. Andrej Trošt, B. Sc.
47. Bogomir Vrhovec, B. Sc.
Technical and administrative staff
48. Tanja Dragojević, B. Sc.
49. Petra Movh, B. Sc.

Note:

* part-time JSI member

BIBLIOGRAPHY

ORIGINAL ARTICLE

1. Mikael Grönkvist, Igor B. Mekjavić, Urša Ciuha, Ola Eiken, "Heat strain with two different ventilation vests during a simulated 3-hour helicopter desert mission", *Aerospace medicine and human performance*, 2021, **92**, 4, 248-256.
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6. Zvezdan Lončarević, Rok Pahič, Aleš Ude, Andrej Gams, "Generalization-based acquisition of training data for motor primitive learning by neural networks", *Applied sciences*, 2021, **11**, 3, 1013.
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8. Andrej Trošt, Marko Jamšek, Nejc Šarabon, Jan Babič, "A system to measure the human body asymmetries using accelerometers", *Elektrotehniški vestnik*, 2021, **88**, 5, 267-272.
9. Urša Ciuha, Alexandros Sotiridis, Tinkara Mlinar, Joshua T. Royal, Ola Eiken, Igor B. Mekjavić, "Heat acclimation enhances the cold-induced vasodilation response", *European journal of applied physiology*, 2021, **121**, 11, 3005-3015.
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12. Tjaša Kunavar, Marko Jamšek, Marie Barbiero, Gunnar Blohm, Daïchi Nozaki, Charalambos Papaxanthis, Olivier White, Jan Babič, "Effects of local gravity compensation on motor control during altered environmental gravity", *Frontiers in neural circuits*, 2021, **15**, 750267.
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Review Article

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Patent

1. Igor Kovač, *Cardan joint*, EP3615823 (B1), European Patent Office, 02. 06. 2021.
2. Anton Umek, Boris Jerman, Mitja Gliha, Anton Kos, Iztok Špan, *Link member for connection of a gripping assembly to a hydraulic crane arm with integrated dynamic weighing assembly*, EP3649071 (B1), European Patent Office, 24. 02. 2021.
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Theses and Mentoring

1. Rok Pahič, *Learning of dynamic movement primitives with deep neural networks:* doctoral dissertation, Ljubljana, 2021 (mentor Aleš Ude).

DEPARTMENT OF SYSTEMS AND CONTROL

E-2

The Department of Systems and Control 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 for supporting the design of control systems, the development of specific measurement and control modules, and the development and construction of complete systems for the control and supervision of machines, devices and industrial processes.

Head:
Asst. Prof. Gregor Dolanc

Basic and applied research in 2021 was devoted to three sub-areas: methodologies for analysis and control system design; tools and building blocks for implementation; and applied research in the priority problem domains.

The first topic addressed the *modelling and identification of nonlinear and complex dynamical systems*. Research activities were pursued in the direction of the method for the simulation of approximated, autoregressive models, utilisation of graphic processing units for the computational acceleration of these models' simulation and hybrid modelling composed of theoretical models and Gaussian-process models. The methods were utilised for the modelling of interdependent atmospheric variables and wastewater treatment plants.

For the Slovenian Research Agency project *Sources, transport and fate of persistent air pollutants in the environment of Slovenia*, most of the activities were comprised of dataset preparation and the research of different computational-intelligence modelling methods for the identification of surrogate models for airpollutants, in particular sulphur dioxide, dispersion modelling. We evaluated different potential identification methods that could be used to develop surrogate models. In making our selection, we placed particular emphasis on the computational burden of the modelling methods.

In the field of smart factories, activities were carried out for the development of a system for non-invasive monitoring and diagnostics of repetitive production processes (Figure 1). The work focused on the development of the methods for segmentation and classification of specific operations of production processes. The methods were tested on test industrial process data and publicly available data sets for time series classification.

Early fault detection and isolation (FDI) is a crucial step during the operation of solid-oxide electrolysis cell (SOEC) stack to mitigate degradation risks. Thus, a FDI tool was developed based on the residuals of the SOEC model. Since faults of the SOEC system components (F1 – temperature sensor error, F2 – fuel/steam leakage, F3 – air leakage) and the SOEC stack itself (F4 – series resistance increment) are the most frequent, a transferable belief model (TBM) was employed to assess the probabilities (P) of the aforementioned faults, as seen in Figure 2, by considering the Kruskal-Wallis p-value of each fault, calculated from the residual time distributions in the fault-free (FF) and fault (F1 – 4) state.

Applied research in the priority problem domains was the second sub-area of our interest. For the Slovenian Research Agency project *Modelling the dynamics of short-term exposure to radiation,* most of the activities were comprised of dataset preparation and the research of different Gaussian-process-based modelling methods for the identification of surrogate models useful for forecasting short-term exposure to radiation. We evaluated different potential identification methods that could be used to develop surrogate models. In making our selection, we placed particular emphasis on the computational burden of the modelling methods.

Figure 1: Classification of production operation segments

In 2021 we continued the work on the ARRS application project *Optimization based control of P2G converter connected to hydro power plant*. The project addresses the potential of green-hydrogen production in a run-of-river hydro power plant. We developed a Simulink hydro power-plant model, containing the physical and economic models of the hydro power plant as the key building blocks. Using the real data for the hydro power-plant timetable and water inflow, we estimated the actual excess of the hydropower that can be used for hydrogen cogeneration. We showed the possibility of a cogeneration of green hydrogen from the surplus water energy, formed during the regular operation of the case-study HPP at the actual water inflows. Using simulations, we showed that the hydro power plant can produce up to 5000 kg of hydrogen from the surplus hydropower per month.

We are cooperating with the *Department of Reactor Physics* at the Jožef Stefan Institute in the project *Stability of nuclear reactors in load following mode of operation*. We implemented and roughly tuned a two-point

Figure 2: Probabilities (P) of faults (F) considering: a) fault-free state (validation data), b) temperature-sensor error, c) fuel / steam leakage, d) air leakage, and e) series resistance increment

nonlinear model of a pressurized-water nuclear reactor in the Matlab/Simulink environment, which is suitable for exploring the control for the load-following mode of operation. In this mode, undesired dynamical phenomena may occur in the reactor, mainly due to the dynamics of xenon that inhibits the nuclear reaction by absorbing neutrons. Due to the reactor construction, this may lead to an asymmetrical vertical distribution and oscillation. We implemented proportional-integral control schemes for the control of the reactor power and its axial offset by manipulating either the boric acid concentration and the main control rods, or the main and auxiliary part-length control rods. We also assessed the possibility of using part-strength control rods.

We started a newly obtained applied research project *Supervisory control system for plant-wide optimization of wastewater treatment plant operation*. The aim of the project is to design a non-model real-time optimization algorithm using extremum-seeking control to optimise clean water production, consumption and production of energy, and reduce operating costs and greenhouse-gas emissions. The activities so far have focused on the preparation of the wastewater treatment benchmark simulation model for performing the research as well as on the analysis of the user requirements.

Following the initiative of the Republic of Slovenia for the establishment and operation of Strategic innovative partnerships within the framework of the Slovenian Smart Specialisation Strategy S4, the *Strategic Innovative Partnership Factories of the Future – SRIP ToP* is also operating. Our department has a very active role in *SRIP ToP* in the management of Control Technologies and in the implementation of its Multi-Annual Action Plan. In 2021 we implemented the plan for the third phase of the Action Plan. One of the important results was the organization of an all-day hybrid conference entitled *Control technologies – technologies that make things work*. The content of this event was included in the series of events *Robotics and Industry 4.0*, which were held at the Digital Centre during the Slovenian Presidency of the Council of Europe.

International R&D projects

The Horizon 2020 project *RUBY – Robust and reliable general management tool for performance and dUraBility improvement of fuel cell stationarY unit*s aims at developing, integrating, engineering and testing a comprehensive and generalized Monitoring, Diagnostic, Prognostic and Control (MDPC) tool capable of improving efficiency, reliability and durability of Solid-Oxide Fuel Cell (SOFC) and Polymer-Electrolyte Fuel Cell (PEMFC) systems for stationary applications. The tool relies on advanced techniques and dedicated hardware and will be embedded in the Fuel-Cell Systems (FCSs) for on-line validation in a relevant operational environment. Therefore, at the end of the project, the RUBY tool will reach a Technology Readiness Level (TRL) equal to TRL 7. It is foreseen that the tool will be ready for engineering, final certification and large-scale production to be embedded within commercial FCSs. In 2021 our team contributed the designs of online diagnostic and prognostic algorithms and a supervisory control system. These will enhance the system lifetime, stack durability, availability, reliability and overall performance with improved efficiency.

Figure 3: INEVITABLE digitalization architecture

The next Horizon 2020 project, coordinated by our department, is *RE-ACTT – REliable Advanced Diagnostics and Control Tools for increased lifetime of solid-oxide cell Technology*.

REACTT is about the development of an HW platform for optimal control, condition monitoring and estimation of the remaining useful life of solid-oxide electrolysis (SOE) and reverse solid-oxide cell (rSOC) systems. These systems are likely to play a major role in the H_2 production at low costs and renewable energy storage. Our team is designing an electronic module for a conceptually new way of stack excitation, diagnostic and prognostic algorithms and a supervisor control module.

In 2021 we continued activities under the H2020 project *INEVITABLE* (Figure 3). An important part of the project activities included project coordination, organization of communication activities and dissemination of interim results. Due to the delays caused by the COVID-19 crisis, we extended the project by half a year and updated the project implementation plan for this reason. In 2021 we also successfully completed the first reporting period. As part of our research work, we continued the development of supportive tools intended for process optimization in the cold rolling of metal sheets at SIJ Acroni. Together with the partners involved, we provided the appropriate infrastructure to collect all the necessary data, which we later analysed and used to develop various predictive models, optimizing rolling recipes and equipment control. In addition, we actively participated in the preparation of design principles for the establishment of a digitalization infrastructure, through which we will introduce the developed technologies into the production environment.

The focus of the *HECAT – Disruptive Technologies Supporting Labour Market Decision Making* project is the development of disruptive data-driven tools for the labour-market characterisation. We are currently at the halfway point of the project. The current results include a decision-support system for an optimal career path discovery, a probabilistic machine-learning model for estimating the probability of exit (time-to-employment) and various derived statistical features that describe the general properties of the labour market such as volatility and liquidity. The next step is the piloting phase, i.e., the integration of the algorithms into the processing infrastructure of the Employment Services of Slovenia.

We are also the partner in the ADRION Interreg project *TRANSCPEARLYWARNING – Establishment of TRANSnational Civil Protection EARLY WARNING system*, aimed at improving the resilience of Adriatic-Ionian territories to natural and man-made risks. The main deliverables of the project are the Civil Protection Early Warning Model, Civil Protection Early Warning Platform and Civil Protection Early Warning System Strategic Plan. We were actively involved in the realisation of the first two of the three above-mentioned deliverables.

Applied work

For our long-term industrial partner *Domel d.o.o.* we completed, in 2021, the development and implementation of a new diagnostic system for the automatic final quality assessment of electric motors on the most complex production line to date. Three completely different types of electric motors are produced on this line, each in many sub-versions. Depending on the currently produced motor type, the diagnostic system sets the required operating parameters and checks the performance of the final product based on the measurements of electrical quantities, vibrations, noise, pressure and special measurements of electronic components. Due to the requirement to achieve a very short test cycle, the system is divided into three consecutive test cells (Figure 4). The system can test around 7000 different types of electric motors daily, and to date more than half a million motors have been tested.

In collaboration with the company *Danfoss Trata, d.o.o.*, we are developing a flow controller where, by the end of the second phase of the multiphase project, we developed in 2021 all the necessary flow control algorithms that work even with delayed measurements of the process. Simulation studies show that we were able to eliminate the overshoot of the regulated flow by predicting the measurement signal and estimate the clogging of the heat exchanger using an additional pressure sensor.

In 2021 the department received an order from the Domel company to develop a new diagnostic system for the end-of-line quality assessment. This is a semi-automatic diagnostic system for a new production line of brushless electric DC motors for vacuum-cleaner units. The system poses a new challenge in terms of digitization, data transfer and operation monitoring as it will be built into a factory in China. The function of the system is to ensure 100% quality of the produced units by means of measuring the electrical and mechanical (pressure, vibration, noise) properties and to monitor fluctuations in the production parameters with the intent to minimize them.

Figure 4: New diagnostic system for automatic final quality assessment of electric motors at Domel d.o.o.

Figure 5: Recipients of the TARAS 2021 Award for the most successful cooperation between the industry and research and development in the field of innovation, development and technologies (Photo: IRT Forum)

Educational and training activities

Some members of the department give 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 Faculty of Industrial Engineering Novo mesto; the University of Nova Gorica; and Jožef Stefan International Postgraduate School.

Some outstanding publications in the past year

1. Žnidarič, Luka, Nusev, Gjorgji, Morel, Bertrand, Mougin, Julie, Juričić, Đani, Boškoski, Pavle. Evaluating uncertainties in electrochemical impedance spectra of solid oxide fuel cells. *Applied energy*, ISSN 0306-2619, 2021, vol. 298, pp. 117101-1-117101-14, doi: 10.1016/j.apenergy.2021.117101. [COBISS.SI-ID 65853187]
2. Nusev, Gjorgji, Morel, Bertrand, Mougin, Julie, Juričić, Đani, Boškoski, Pavle. Condition monitoring of solid oxide fuel cells by fast electrochemical impedance spectroscopy : a case example of detecting deficiencies in fuel supply. *Journal of power sources*, ISSN 0378-7753, 2021, vol. 489, pp. 229491-1-229491-10, doi: 10.1016/j.jpowsour.2021.229491. [COBISS.SI-ID 48196099]

3. Boškoski, Pavle, Perne, Matija, Rameša, Martina, Mileva Boshkoska, Biljana. Variational Bayes survival analysis for unemployment modelling. *Knowledge-based systems*, ISSN 0950-7051. [Print ed.], 11 Oct. 2021, vol. 229, [article no.] 107335, str. 1-11, doi: 10.1016/j.knosys.2021.107335. [COBISS.SI-ID 71383555]

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5. Krivec, Tadej, Kocijan, Juš, Perne, Matija, Grašič, Boštjan, Božnar, Marija, Mlakar, Primož. Data-driven method for the improving forecasts of local weather dynamics. *Engineering applications of artificial intelligence*, ISSN 0952-1976. [Print ed.], 2021, vol. 105, pp. 104423-1-104423-14, doi: 10.1016/j.engap-pai.2021.104423. [COBISS.SI-ID 74917635]

Some outstanding achievements in the past year

1. Our department and Danfoss Trata d.o.o. received the *TARAS Award* for the most successful cooperation between the industry and the research and development in the field of innovation, development and technology in 2021, namely, for the development of intelligent motor drives that enable the optimization of entire district heating and cooling networks (Figure 5).

2. Our associate Martin Brešar from the Faculty of Mathematics and Physics in Ljubljana received the *Prešeren Award 2021* for his master's thesis entitled *Direction of Coupling in Nonlinear Systems.*

3. In 2021 we received an order from Domel d.o.o. to develop a new diagnostic system for the final quality assessment of electric motors to be installed at their factory in China.

Awards and Appointments

1. Danfoss Trata and Department of Systems and Control at the Jožef Stefan Institute are the recipients of the TARAS award for 2021 for the development of intelligent motor drives, which is presented by the IRT Industrial Forum, the organiser of the main professional event for Slovenian industry, to recognise the most successful cooperation between business and the research and development environment in the field of innovation, development and technology, Portorož, Slovenia

VISITORS FROM ABROAD

1. Prof. Ivana Palunko, University of Dubrovnik, Dubrovnik, Croatia, 14–17 December 2021
2. Dr Domagoj Tolić, Rochester Institute of Technology Croatia, Dubrovnik Croatia, 14–17 December 2021
3. Dr Rade Garić, University of Dubrovnik, Dubrovnik, Croatia, 14–17 December 2021

INTERNATIONAL PROJECTS

1. H2020 - RUBY; Robust and Reliable General Management Tool for Performance and Durability Improvement of Fuel Cell Stationary Units
   Prof. Đani Juričić
   European Commission
2. H2020 - HECAT; Disruptive Technologies Supporting Labour Market Decision Making
   Asst. Prof. Pavle Boškoski
   European Commission
3. H2020 - INEVITABLE; Optimization and Performance Improving in Metal Industry by Digital Technologies
   Dr. Dejan Gradišar
   European Commission
4. H2020 - REACTT; REliable Advanced diagnostics and Control Tools for increased lifetime of solid oxide cell Technology
   Prof. Đani Juričić
   European Commission
5. TRACE - Phylogenetic Reconstruction Using Gaussian Processes
   Prof. Juš Kocijan
   Slovenian Research Agency

RESEARCH PROGRAMME

1. Program systems and control
   Prof. Đani Juričić

R&D GRANTS AND CONTRACTS

1. Degradation monitoring and performance optimisation of solid oxide electrolysis cells
   Prof. Đani Juričić

2. STRAP - Sources, TRansport and fate of persistent Air Pollutants in the environment of Slovenia
   Prof. Juš Kocijan
3. Optimization based control of P2G converter connected to hydro power plant
   Asst. Prof. Gregor Dolanc
4. Stability of nuclear reactors in load follow mode of operation
   Dr. Boštjan Pregelj
5. Modelling the Dynamics of Short-Term Exposure to Radiation
   Prof. Juš Kocijan
6. Supervisory control system for plant-wide optimization of wastewater treatment plant operation
   Dr. Darko Vrečko
7. Circular 4.0: Digital technologies as enabler to foster the transition to the circular economy bythe SME in the Alpine Space area
   Dr. Miha Glavan
   Government Office of the Land of Salzburg

NEW CONTRACTS

1. Development of end-of-line quality inspection system for brushless motor types 712, 720 and 759 for line ML15
   Asst. Prof. Gregor Dolanc
   Domel, d. o. o.
2. Optimization based control of P2G converter connected to hydro power plant
   Asst. Prof. Gregor Dolanc
   Hidroelektrarne na spodnji Savi, d. o. o.
3. Modelling the Dynamics of Short-Term Exposure to Radiation
   Prof. Juš Kocijan
   Krško Nuclear Power Plant

STAFF

Researchers

1. Asst. Prof. Pavle Boškoski
2. **Asst. Prof. Gregor Dolanc, Head**
3. Dr. Samo Gerkšič
4. Dr. Miha Glavan
5. Dr. Giovanni Godena
6. Dr. Dejan Gradišar
7. Dr. Nadja Hvala
8. Dr. Vladimir Jovan
9. Prof. Đani Juričić
10. Prof. Juš Kocijan
11. Dr. Marko Nerat
12. Asst. Prof. Matija Perne
13. Dr. Janko Petrovčič
14. Dr. Boštjan Pregelj
15. Asst. Prof. Damir Vrančić
16. Dr. Darko Vrečko

Postgraduates

17. Martin Brešar, B. Sc.
18. Žiga Gradišar, B. Sc.
19. *Dr. Tomaž Kos, left 01.06.21*
20. Tadej Krivec, B. Sc.
21. Jernej Mlinarič, B. Sc.
22. Gjorgji Nusev, B. Sc.
23. Žiga Stržinar, B. Sc.
24. Luka Žnidarič, B. Sc.

Technical officers

25. Stanislav Černe, B. Sc.
26. Primož Fajdiga, B. Sc.
27. David Jure Jovan, B. Sc.

Technical and administrative staff

28. Maja Janežič, B. Sc.
29. Miroslav Štrubelj

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6. Viktor Andonovic, Pavle Boškoski, Biljana Mileva Boshkoska, "Estimating client's job-search process duration", In: *IS 2021, Slovenian Conference on Artificial Intelligence, 8. October 2021, Ljubljana, Slovenia*,

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DEPARTMENT FOR ARTIFICIAL INTELLIGENCE E-3

The Artificial Intelligence Laboratory (http://ailab.ijs.si/) is concerned mainly with the research and development of information technologies with an emphasis on artificial intelligence. Our main areas of research are: data analysis with an emphasis on text, web and cross-modal data, scalable real-time data analysis, machine learning, analysis and modelling of large networks, visualization of complex data, semantic technologies, language technologies, reasoning methods and knowledge management. The Artificial Intelligence Laboratory has employees and students with an international background and expertise in different areas of artificial intelligence. In addition to publishing their research results in international publications and presenting their work at international events, our researchers have also developed numerous software tools for multimodal data analysis. These tools include: Text-Garden, a suite of text mining tools; OntoGen (http://ontogen. ijs.si/), a tool for ontology learning; Document-Atlas (http://docatlas.ijs.si/), a tool for complex visualization; Atlas of Slovenian Science (http://scienceatlas.ijs.si/), a web portal for analyzing the scientific community; Enrycher (http://enrycher.ijs.si/), a system for semantic enrichment of textual data; SearchPoint (http://searchpoint.ijs.si/), a portal for visual and contextualized Web browsing; OntoPlus, a methodology for semi-automatic ontology extension; Contextify (http://contextify. net/), a tool for contextualized e-mail and contact management; Qminer (http://qminer.ijs.si/), a data analytics platform for processing large-scale real-time streams containing structured and unstructured data; NewsFeed (http://newsfeed.ijs.si/), a clean, continuous, real-time aggregated stream of semantically enriched news articles from RSS-enabled sites across the world; EventRegistry (http://eventregistry.org/), a system for identifying world events in news media including a DarkNET component of Event Registry (https://eventregistry.org/); Wikifier (http://wikifier.org), a system for document annotation with links to relevant Wikipedia concepts; StreamStory (http://streamstory. ijs.si), an exploratory data stream analysis tool offering an alternative type of visualization by representing the multivariate data stream using a Markovian model; Videolectures Explorer (http://explore.videolectures.net/), a tool enabling users to search through video lectures and find similarities between them; EDSA dashboard (http://jobs.videolectures.net/), a tool aggregating demand data (job postings around Europe) and supply data (training materials) in data science;

Head:

Prof. Dunja Mladenić

nextPin (http://traffic.ijs.si/NextPin/?user=demo), a system for the analysis of time varying data of geographic locations, Connection tool (http://connection.ijs.si), a tool based on Event Registry news data, which allows a user to follow business and personal named entities in time and establish broad relations between named entities (based on shared Wikipedia concepts from news articles) as well as to view the changes in these relations; Graph Based Analytics (http:// gba.ijs.si), a service for business relation identification from text which enables identification of business relations, such as mergers & aquisitions, bankruptcy, earnings, dividends, etc., based on sentence level; streamfusion, universal system for the preprocessing of heterogenous stream data; ELEXIS ER (http://er.elex.is/) a lexicography-adapted version of Event Registry; a public procurement anomaly detection tool (http://tbfy.ijs.si/), a service for processing, analysing and searching through the environmental legal documents (http://envirolens.ijs.si/); Infominer, a tool for interactive data analysis (https://infominer.ijs.si/); Water Observatory (http://naiades.ijs. si/); MultiCOMET (https://multicomet.ijs.si/), a system for automatic generation of commonsense descriptions; Smell Tracker (https://odeuropa.ijs.si/); EUJapan Observatory (https://eujapan.ijs. si/), monitoring the use of AI in manufacturing, and StreamStory (http://atena.ijs.si:8080/), a tool for converting time series into system states. The laboratory's strategy is to combine scientific excellence with strong industrial collaboration, enabling the transfer of research results into real-world business environments.

The IRCAI was officially launched on 29 March 2021. Its virtual conference took place on 29–30 March 2021.

On 29–30 March 2021 the International Research Center on Artificial Intelligence under the auspices of **UNESCO – IRCAI** held its official launch with 1083 registered participants from 123 countries. The center organized

and co-organised 38 events, reached 110 companies and engaged in 35 different national and international projects. In 2021 the IRCAI setup a network to strengthen AI research centres of excellence around the world, aiming to facilitate their collaboration and networking to increase the research capacity in AI and sustainable development. This initiative is also intended to contribute to the development of ethical and trustworthy AI, as described in the UNESCO Recommendation, to which the experts of the IRCAI network contributed. In 2021 the IRCAI held extensive discussions with 40 core partners.

The Ministry of Foreign Affairs of the Republic of Slovenia, the Slovenian Presidency and IRCAI joined forces to organize 10 events in close cooperation with Slovenian embassies and other permanent missions in 9 countries around the world. The events were accompanied by the awarding of the IRCAI Award, which recognizes the valuable work of individual researchers, developers or educators who have demonstrated results and impact of applying AI to achieve one of the seventeen UN SDGs. In 2021 the IRCAI issued a call entitled *Top 100 to collect solutions in AI with global relevance in sustainable development*. Participating applicants came from all five geographic regions: Africa, Europe and the Americas, Asia and the Pacific, and the Middle East.

The IRCAI was asked, through the Slovenian government, by the DG EAC to host the main event of the Digital Education Hackathon (DigiEduHack), a flagship initiative of the Digital Education Action Plan, during the Slovenian Presidency of the European Council (July–December 2021). The hackathon attracted 2058 participants from 71 countries worldwide, and the event successfully promoted the link between sustainability and digital education. 51 solutions were created by DigiEduHackers aged 10 to 60+ and uploaded to digieduhack.com. The three winners of the DigiEduHack 2021 Global Award will be announced in 2022. A Slovenian hackathon was also jointly organized by the IRCAI and GreenHack consortia.

Members of the Department for Artificial Intelligence successfully continued to participate within the EU, in national and regional projects. In the last 19 years, the AILAB participated in 80 EU projects, of which 3 were concluded in 2021 and 11 were still ongoing. The AILAB also participated in 5 national projects.

In 2021 in the area of **statistical data modelling and machine learning**, we continued work within **CogLo**, **Naiades** and **FACTLOG** and began work within the EU project **STAR**. The EU H2020 project **Cog-Lo** *(Cognitive Logistics)* started in June 2018. The aim of the project is to design and develop an intelligent logistics platform with cognitive services for postal operators/infrastructure. The project focuses on observing postal infrastructure as an object in time, with its dynamic parcel (packets) flow being driven through basic infrastructural tools. The cognitive-services platform will utilize infrastructure data to build a digital representation and dynamically route/allocate assets for process performance optimization. In the scope of the project, we have designed a methodology for building a digital representation of a physical infrastructure, methodology for optimization of resources on the graph distribution, and methodology for large graph processing with clustering. Algorithms for the assessment of logistics events in real time enable the assessment of the optimal response to ad-hoc requests for interventions in the logistics parcel delivery. The analytical pipeline was integrated and tested in a demo solution. The integrated solution was presented and implemented in real-case scenarios in three different test-bed sites, namely: Slovenia-Croatia (the cross-border region from Brežice to Zagreb), Greece (Athens) and the Ekol logistics chain with a pilot from Italy (Trieste) to East Europe (Poland). In the scope of the project, a cognitive adviser tool was developed as the main agent monitoring events in the infrastructure in real-time and creating interventions for the process optimization.

Within the EU H2020 project **Naiades** *(A holistic water ecosystem for digitisation of urban water sector)*, our team is responsible for (1) monitoring the water supply system, by presenting water-supply time series data through identified system states in order to acquire additional insights into the system behavior; (2) identifying and predicting anomalies in the data, aggregated through various water-related systems (e.g., water-supply system, wastewater system); (3) making short-term (up to 10 days in advance) predictions of water consumption for a given settlement and (4) creating consumer confidence heatmaps in relation to the water supply for a given settlement and applying predictive models that will help us obtain additional insights into their future changes. In 2021 we conceptualized and delivered all of the core components, upon which AI services will be built. We identified and
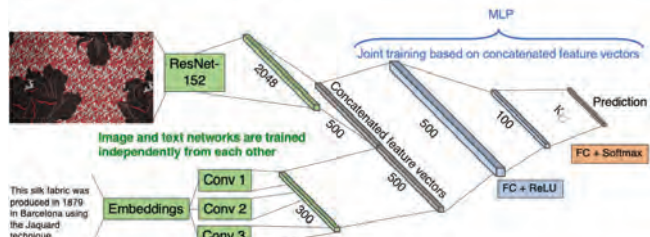
Figure 1: SILKNOW semantic search engine across the history of silk using deep learning

tested data sources, data models as well as underlying architectures for the technical solutions. We also delivered all of the key components for the final solutions. In coordination with the Naiades consortium, one of our tasks was redefined into building a Global Water Observatory.

The goal of the EU Horizon 2020 project **FACTLOG** *(Energy-Aware Factory Analytics for Process Industries)* is to support the process industry through the development of digital twins. As a digital representation of a factory supported by analytics systems, a digital twin supports functions such as: raising an alarm when encountering an anomaly, planning the optimal order of production and appropriately setting the parameters of production machinery. Together with the partners, we designed a framework, in which machine-learning models work together with domain expert models and optimisation algorithms to solve industry problems. Our main contributions are the software libraries for forecasting industry system states from data streams and the detection of anomalies in data streams. The methods are being tested within industry pilots, the main partners being: JEMS, a Slovenian company processing waste into fuel, and Tüpraş, a Turkish oil refinery. The EU Horizon 2020 project **STAR** *(Safe and Trusted Human Centric Artificial Intelligence in Future Manufacturing Lines)* began in January 2021, introducing novel AI technologies for dynamic and unpredictable manufacturing environments. AI systems are already used to improve the automation of production in the manufacturing sector, however, the STAR project is aiming to also improve trustworthiness when the systems are replacing human tasks in dynamic operations. The project is aimed to research and integrate leading-edge technologies such as active learning, simulated reality, explainable AI, human-centric digital twins, advanced reinforcement learning and cyber-defense mechanisms.

In the area of **data stream analysis**, we continued to develop the *Platform for Anti-Money Laundering* and *Counter Financing of Terrorism* as one of the 15 fintech pilots of flag ship project **INFINITECH** (*Tailored IoT & BigData Sandboxes and Testbeds for Smart, Autonomous and Personalized Services in the European Finance and Insurance Services Ecosystem*); it includes 15 different pilots in the fintech domain, one of which focuses on the development of an analytical platform for Anti-Money Laundering and Counter Financing of Terrorism (PAMLS) for supervising financial institutions, where our partner is the Bank of Slovenia. Only two partners are involved in the development of this pilot – the Bank of Slovenia as the content partner and the end user and the JSI AILAB as the technology partner. The developed PAMLS methods were verified against the facts of pseudoanonimized historical data. As the technology partner, we contributed three components: (1) pseudo-anonymizer – a service for data pseudo-anonymization, and two PAMLS tools: (2) the second version of the Risk Assessment Tool and (3) the first version of the Screening Tool, which showed extremely good results in the validation test. The project CyberSANE (*Cyber Security Incident Handling, Warning and Response System for the European Critical Infrastructures*) started in 2019, aiming to increase the security and resilience of the European Critical Information Infrastructure (CII). As part of the project, we are developing a CyberSANE platform to help professionals in organizations deal with cyber incidents. In 2021 we continued working with partners to develop the technology for capturing and analyzing structured and unstructured data from the so-called dark web as well as from media articles. The data captured from the news and dark web will be used in the DarkNET component of the CyberSANE platform and will enable the creation of reports and alerts on detected cyber threats.

We successfully concluded two EU H2020 projects: Silknow (Silk Heritage in the Knowledge Society: from punched cards to big data, deep learning and visual/tangible simulations) and Fintech (a FINancial supervision and TECHnology compliance training programme)

In the areas of **text and network analysis and language technologies**, we successfully concluded the EU H2020 project **SILKNOW** (*Silk Heritage in the Knowledge Society: from punched cards to big data, deep learning and visual / tangible simulations*). To enable a semantic view on the texts describing cultural heritage, we developed a multilingual text-annotation service that enables the annotation of texts with Wikipedia concepts and with terms from our domain-specific thesaurus http://wikifier.org/silknow.html. To enrich the available cultural heritage data, we developed methods for the extraction of relevant values from texts, such as the number of sections on silk based on its textual description, and methods for the prediction of the missing properties of the existing semantic fields, such as the production place of a historic artifact. These were evaluated in English, French, Spanish and Italian texts. In the final stages we developed several approaches to a multimodal prediction of missing artifact properties by integrating the text analysis and image analysis.

The H2020 **ODEUROPA** project (*Negotiating Olfactory and Sensory Experiences in Cultural Heritage Practice and Research*) intends to apply state-of-the-art AI techniques to cultural heritage text and image datasets spanning four centuries of European history, to find and trace how 'smell' was expressed in different languages, with what places it was associated, what kinds of events and practices it characterized, and to what emotions it was linked. In 2021 the Odeuropa partners started building the project infrastructure, organizing and participating in smell related events (workshops, conferences, dissemination to public), discovering smell textual and visual resources. In particular, the AILAB contributed to the extraction and annotation of the historical documents in Slovene with a smell related annotation schema, and to the development of the odor ontology. We created a Smell Tracker tool,

which allows the exploration of the "odor" aspect in semantically annotated textual resources, providing a number of visualizations and statistics related to the cross-lingual and multi-lingual documents. We developed guidelines for emotion annotations of smell related contents and created the first models for detecting emotions related to smells.

We also continued to coordinate the EU Horizon 2020 project **ELEXIS** (*European Lexicographic Infrastructure*) that started in February 2018. The aim of the project is to integrate, extend and harmonize national and regional efforts in the field of lexicography, both modern and historical, with the goal of creating a sustainable infrastructure, which will (1) enable efficient access to high-quality lexical data in the digital age, and (2) bridge the gap between more advanced and lesser-resourced scholarly communities working on lexicographic resources. In 2021 in addition to project management activities, we continued to maintain the project website and upgraded the Elexifinder tool.

Figure 2: Top: CogLo analytics tested in a simulated environment; bottom: CogLo architecture – cognitive adviser integrated with SIoT

We continued to improve and test the Elexifier tool: over 200 dictionaries were converted and integrated into the database. We launched the first version of the service for linking semantic data in dictionaries and started work on the Dictionary Matrix. We also further developed the Lexonomy system, which we use for the preparation of dictionaries. In particular, we have been developing building blocks for a better visualisation of dictionaries.

As a part of the H2020 EU Marie Skłodowska-Curie ITN project **CLEOPATRA** (*Cross-Lingual Event-Centric Open Analytics Research Academy*), two employed researchers, ESR-11 and ESR-12, published six research papers, completed their first secondment and attended several CLEOPATRA meetings. Their secondments were hosted by UoL (University of London) and UvA (University of Amsterdam), respectively. During Cleopatra Hackathons, they contributed towards the creation of the second version of the OEKG (Open-Event Knowledge Graph) and the CKPP (CLEOPATRA Knowledge Processing Pipeline). Their work during Research and Development events were focused on collaborative research, while their work during Learning Week events were centered on advanced computer science, interdisciplinary topics and professional development. They also participated in the Innovation Week and Career Fair, which introduced entrepreneurship and start-up companies through courses, tutorials and workshops. The area of **text and network analysis and language technologies** also included work in national and regional projects. In 2021 we continued our work on the project **Development of Slovene in a Digital Environment (RSDO)**, which is co-financed by the Republic of Slovenia and the European Union under the European Regional Development Fund. The operation is carried out under the Operational Programme for the Implementation of the EU Cohesion Policy 2014–2020. The results include new language resources, Slovene processing tools and applications (upgrading of text corpora, speech recognition, semantic technologies, machine translation, terminology portal, maintenance of the Language Technology Centre – CLARIN). In the second year of the project, we completed intensive student work on the annotation of the Sloleks lexicon and the ssj500k corpus. We also continued to develop the MultiCOMET tool. This is a model that generates contextual assertions according to the sentence being typed. It includes the conditions and consequences of what is typed, generating a graphical representation of the assertions. A deep neural network parses the input and makes a conclusion based on the context and influences. The ATOMIC database was translated for this tool.

In 2021 the **MARCELL** project ended. Its main objective was to provide comparable segments (near-translations) of national legal texts (laws, regulations, rules) from seven countries – Croatia, Hungary, Poland, Slovakia, Bulgaria, Romania and Slovenia. National legal texts were not automatically available on CEF.AT, but machine translators can be improved if they have access to legal texts enriched with metadata (lemmatisation, linguistic tagging, tagging with IATE terms and EUROVOC descriptors). In 2021 the final JSI activities included a semantic micro-compilation and an improvement of corpus annotations and document classification algorithms. The main objective of the **CurliCat** project (**Curated Multilingual Language Resources for CEF AT Action**) is to collect curated databases for the seven consortium languages (Bulgarian, Croatian, Hungarian, Polish, Romanian, Slovak, Slovene) in order to improve the European Commission's machine translator. In 2021 we started to develop a text anonymisation system for all 7 languages.

The **Federated eTranslation TermBank Network (FedTerm)** project aims at developing federated terminology collections (nodes) where users can manage and share their terminology with each other and search for terms in
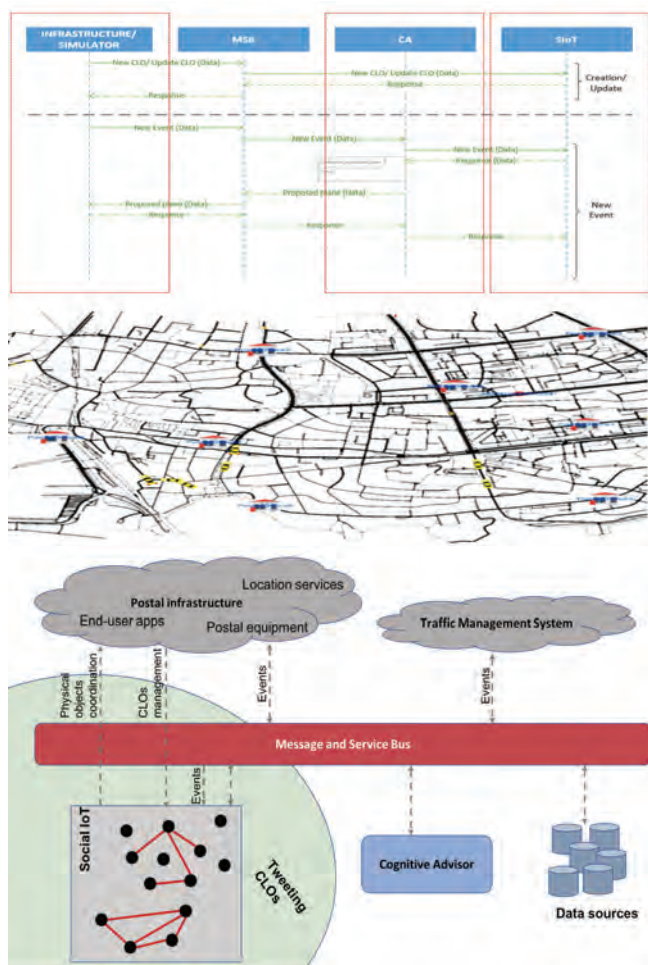
private and publicly available terminology collections. The project is developing a network that allows organisations and institutions in the EU to locally deploy individual eTranslation TermBank federated nodes, linked to the central federated node (the eTranslation TermBank) and regularly synchronise terminology changes. The project will cover all EU official languages as well as Norwegian and Icelandic, focusing on the partner languages (Latvian, Danish, Icelandic, Estonian, Lithuanian, Slovene, German and Swedish). We are also participating in projects within the **ELRC (European Language Resource Coordination)**. It manages, maintains and coordinates the relevant language resources in all official languages of the EU and CEF (Connecting Europe Facility) associated countries. These activities will help to improve the quality, coverage and performance of automated translation solutions in the context of current and future CEF digital services. In 2021 we took part in the initiative **ELG (European Language Grid)**, which will contribute to the emergence of a truly connected, language-crossing Multilingual Digital Single Market by providing powerful multilingual, cross-lingual and monolingual technologies. We also participate in the **European Language Equality (ELE)** project, developing a strategic-research, innovation and implementation agenda as well as a roadmap for achieving full digital language equality in Europe by 2030. In 2021 we signed a cooperation agreement with the language technology company Tilde, the Language Technology Laboratory at the Faculty of Computer Science, University of Latvia, and the Centre for Language Resources and Technologies, University of Ljubljana. By signing the agreement, these institutions recognise the importance of promoting the development of the Latvian and Slovene languages in the field of digital technologies, as well as international cooperation and the exchange of competences, knowledge and data in this field. Together with the Department of Knowledge Technologies (E8), we continued to lead the Slovenian research infrastructure **CLARIN.SI**, which provides easy publication and sustainable access to digital language data for scholars in the humanities and social sciences. In addition to providing support for the CLARIN.SI repository, we also contributed various types of data (lexical resources, corpora, training corpora) and technologies for Slovene language processing.

In the area of **semantic technologies**, the AILAB runs the national project **Causalify**, within which we developed a theoretical model and, based on that, several approaches in different domains. We developed an approach to predicting the future development of scientific research based on scientific publications from the past two centuries. On the problem of text analysis, we developed a model for understanding texts using agent-based models that was validated on a short story. To analyse the cause and effect of personal activities, we developed a system for automatic generation of commonsense descriptions *MultiCOMET.* In the financial domain, we developed an approach to characterizing financial markets from the event driven perspective.

In the area of **knowledge management**, the group's main focus is on research and development using methods and tools from the broader artificial-intelligence area in real business settings. In 2020 we continued with the **Water4Cities** (*Integrated Surface and Groundwater Management for Sustainable Urban Development*) project under the EU Horizon 2020 Marie Sklodowska Curie RISE project, together with the Centre for Knowledge Transfer in IT. We continued with the data analysis of the groundwater, river and stormwater flow data for the Ljubljana aquafier as well as the water quality and consumption on the Greek island of Skiathos. We continued with the development of the models and platform that will allow us to monitor the optimal water management in real time. In 2021 we continued with the publication of regular webinars, available at Videolectures.NET subpage - http://videolectures.net/water4cities/.

The EU Horizon 2020 project **HumanE-AI-Net** (*Making artificial intelligence human-centric*) is a continuation of **HumaneAI** (*Toward AI Systems that Augment and Empower Humans by Understanding us, our Society and the World around us*), which brings together the leading European research centres, universities and industrial enterprises into a network of Centres of Excellence. The leading global artificial intelligence (AI) laboratories will collaborate with the key players in areas such as human-computer interaction, cognitive, social and complexity sciences. The project participants are looking forward to driving researchers out of their narrowly focused fields and connect them with the people exploring AI on a much wider scale. The challenge is to develop robust, trustworthy AI systems that can 'understand' humans, adapt to complex real-world environments and interact appropriately in complex social settings. HumanE-AI-Net will lay the foundations for designing the principles for a new science that will make AI based on European values and closer to Europeans.

The EU Horizon 2020 project **FIN-TECH** (*A FINancial supervision and TECHnology compliance training programme*) was successfully completed in 2021. The aim of the project was to develop a program for the exchange of knowledge in the financial environment. The project incorporated 24 partners covering all 28 European countries, plus Switzerland. Within this project, our department closely collaborated with the Bank of Slovenia in order to provide insight and knowledge in the technical aspects of this rapidly developing field. In 2021 we prepared an online workshop on Blockchain technology. The H2020 **EU-Japan.AI** project (*Advancing Collaboration and Exchange of Knowledge between the EU and Japan for AI-Driven Innovation in Manufacturing*) aims to establish and stimulate a long-term cooperation between the EU and Japan in areas relevant for AI-driven innovation in manufacturing and digital industry by implementing a platform-based approach, connecting all the

relevant stakeholders, and by promoting the use of modern, online-driven awareness approaches. The project is collecting data about relevant events, projects, organizations and opportunities in the EU and Japan in the area of AI in manufacturing. This information is published on a web portal, together with other relevant resources useful for connecting partners from both regions and to foster cooperation among them. Within the project we are developing the EUJapan Observatory, which is currently automatically collecting and analyzing research papers in the AI-related area and media reports on AI-related activity from global news media. In the following months, we will implement the data collection and analysis of jobs and skills market in the AI-related area, research projects and open source projects. We are also preparing AI policies visualization and an analysis for both regions. The goal of the project **KaUČ**: *Improving the Quality of Slovene Textbooks* is to develop quality metrics for Slovene primary and secondary school textbooks to be used during their certification and evaluation. The research group will develop the prototype of an automatic web-based tool, which will allow the evaluation of textbooks based on their textual and pictorial properties. The tool will support the decision-making process for the selection of appropriate textbooks. In 2021 we continued developing the tool for scoring the text readability in Slovene.

The promotion of science is continually present in the efforts of our department. In 2021 members of the Artificial Intelligence Laboratory were very active in promoting artificial intelligence and science in general.

- Marko Grobelnik gave over 5 interviews to various media speaking about topics such as: IRCAI Centre, AI and ethics, and various EU projects
- Dunja Mladenić moderated the Bled Strategic Forum Panel on Digital Europe
- Marko Grobelnik gave the talk "Digital Twin technology may save lives and solve the biggest challenges facing humanity"
- Marko Grobelnik was invited to the Open Knowledge Day
- Alenka Guček gave an interview to the Delo newspaper – "From cell biology to data visualization"

Together with the Centre for Knowledge Transfer in Information Technologies (CT3), we continued to use the Videolectures.NET portal to promote artificial intelligence, the Jožef Stefan Institute and Slovenian research in general. We are also among the main organizers and supporters of the annual national ACM Computer Science Competition for secondary-school students; in 2021, 176 students from 27 schools participated in the competition. We were also active in promoting women in science providing a virtual exhibition about female PhD holders in the area of computer science and electrical engineering in Slovenia. We are also constantly updating our publicly available resources related to women-in-science issues and international news (http://ScienceWithArt.ijs.si/).

Gender equality is the topic of the H2020-CSA project **Athena**, in which we are collaborating with other partners, aiming to unlock research potential and remove barriers to the recruitment, retention and career progression of female researchers, lowering gender imbalances in decision-making processes and generating a cultural change needed to avoid gender bias and discriminatory practices through the implementation of gender equality plans (GEPs). To ensure a systemic institutional change, the project plans to conduct an assessment of the procedures and practices already in place in partner organizations, together with an analysis of the national legislation and policy frameworks. In parallel, it will put in place a participatory process aimed, on the one hand, to understand the needs and preferences of the stakeholders and, on the other hand, to train them on selected topics related to gender. As the final result, each partner organization will draft and implement its specific GEP.

In 2021 we were very actively involved in submitting new project proposals, particularly within the EU Horizon Europe Programme. Three new EU projects began in 2021: *STAR, EUJapanAI* and *ODEUROPA,* while we also obtained funding for a Eurostat project and a national CRP project. We continue with our successful efforts to include the Slovenian industry into the European research area where, over the last 19 years, we contributed to the list of numerous companies participating in the EU projects.

Some outstanding publications in the past year

1. Torkar, Miha, Mladenić, Dunja. Characterizing financial markets from the event driven perspective. *Applied Network Science*. 2021, vol. 6, 74-1-74-37. ISSN 2364-8228. DOI: 10.1007/s41109-021-00417-z. [COBISS.SI-ID 85486339], [SNIP]

2. Rožanec, Jože M., Kažič, Blaž, **Škrjanc**, Maja, Fortuna, Blaž, Mladenić, Dunja. Automotive OEM demand forecasting: a comparative study of forecasting algorithms and strategies. *Applied Sciences*. 2021, vol. 11, no. 15, 6787-1-6787-19. ISSN 2076-3417. DOI: 10.3390/app11156787. [COBISS.SI-ID 85590019], [JCR, SNIP, WoS until 19 January 2022: total citations (TC): 3, citation index (CI): 1, citation index per author (CIAu): 0.20, Scopus until 19 December 2021: total citations (TC): 2, citation index (CI): 0, citation index per author (CIAu): 0.00]

3. Rožanec, Jože M., Trajkova, Elena, Kenda, Klemen, Fortuna, Blaž, Mladenić, Dunja. Explaining bad forecasts in global time series models. *Applied Sciences*. 2021, vol. 11, no. 19, 9243-1-9243-23. ISSN 2076-3417. DOI:

10.3390/app11199243. [COBISS.SI-ID 85587971], [JCR, SNIP, WoS until 19 January 2022: total citations (TC): 1, citation index (CI): 1, citation index per author (CIAu): 0.20, Scopus until 1 January 2022: total citations (TC): 1, citation index (CI): 1, citation index per author (CIAu): 0.20]

4. Pita Costa, João, Stopar, Luka, Grobelnik, Marko, Mladenić, Dunja, Novalija, Inna, et al. NewsMeSH: a new classifier designed to annotate health news with MeSH headings. *Artificial Intelligence in Medicine*. [Printed ed.]. 2021, vol. 114, 102053-1-102053-11, graphs, tables. ISSN 0933-3657. DOI: 10.1016/j.artmed.2021.102053. [COBISS.SI-ID 55329539], [JCR, SNIP, WoS until 25 February 2022: total citations (TC): 1, citation index (CI): 1, citation index per author (CIAu): 0.08, Scopus until 5 March 2022: total citations (TC): 1, citation index (CI): 1, citation index per author (CIAu): 0.08]

5. Matošević, Goran, Dobša, Jasminka, Mladenić, Dunja. Using machine learning for web page classification in search engine optimization. *Future Internet*. 2021, vol. 13, no. 1, 9-1-9-20. ISSN 1999-5903. DOI: 10.3390/fi13010009. [COBISS.SI-ID 46930691], [SNIP, WoS until 20 August 2021: total citations (TC): 2, citation index (CI): 2, citation index per author (CIAu): 0.67, Scopus until 13 September 2021: total citations (TC): 4, citation index (CI): 4, citation index per author (CIAu): 1.33]

6. Swati, J., Mladenić, Dunja, Erjavec, Tomaž. EveOut: an event-centric news dataset to analyze an outlet's event selection patterns. *Informatica: an international journal of computing and informatics*. [Printed ed.]. 2021, vol. 45, no. 7, 25–30. ISSN 0350-5596. DOI: 10.31449/inf.v45i7.3410. [COBISS.SI-ID 95368963], [SNIP]

7. Zajec, Patrik, Rožanec, Jože M., Trajkova, Elena, Novalija, Inna, Kenda, Klemen, Fortuna, Blaž, Mladenić, Dunja. Help me learn! Architecture and strategies to combine recommendations and active learning in manufacturing. *Information*. 2021, vol. 12, no. 11, 473-1-473-27. ISSN 2078-2489. DOI: 10.3390/info12110473. [COBISS.SI-ID 87582723], [SNIP, Scopus until 1 March 2022: total citations (TC): 1, citation index (CI): 1, citation index per author (CIAu): 0.14]

8. Sittar, Abdul, Mladenić, Dunja, Grobelnik, Marko. Analysis of information cascading and propagation barriers across distinctive news events. *Journal of Intelligent Information Systems*. 2021, 34 pp., ilustr. ISSN 0925-9902. DOI: 10.1007/s10844-021-00654-9. [COBISS.SI-ID 87232003], [JCR, SNIP]

9. Kosem, Iztok, Bálint **Čeh**, Júlia, Ponikvar, Primož, Zaranšek, Petra, Kamenšek, Urška, Koša, Peter, Gróf, Annamária, Böröcz, Nándor, Harmat Császár, Jolanda, Szíjártó, Imre, **Šantak**, Borut, Gantar, Polona, Krek, Simon, Roblek, Rebeka, Zgaga, Karolina, Logar, Urban, Pori, Eva, Arhar Holdt, **Špela**, Gorjanc, Vojko. Comprehensive Slovenian-Hungarian Dictionary 1.0. Ljubljana: Centre for Language Resources and Technologies, University of Ljubljana, 2021. CLARIN.SI data & tools. http://hdl.handle.net/11356/1453. [COBISS.SI-ID 97283331]

10. **Čibej**, Jaka, Arhar Holdt, **Špela**, Dobrovoljc, Kaja, Krek, Simon. Frequency lists of character-level n-grams from the GOS 1.0 corpus 1.1. Ljubljana: Jožef Stefan Institute, 2021. CLARIN.SI data & tools. http://hdl.handle.net/11356/1363. [COBISS.SI-ID 53370883]

11. Krek, Simon, Gantar, Polona, Kosem, Iztok, Dobrovoljc, Kaja, Arhar Holdt, **Špela**, **Čibej**, Jaka, Laskowski, Cyprian Adam, Klemenc, Bojan, Krsnik, Luka. Frequency lists of collocations from the Gigafida 2.1 corpus. Ljubljana: Centre for Language Resources and Technologies, University of Ljubljana, 2021. http://hdl.handle.net/11356/1415. [COBISS.SI-ID 58622467]

12. **Čibej**, Jaka, Arhar Holdt, **Špela**, Dobrovoljc, Kaja, Krek, Simon. Frequency lists of word-level n-grams from the GOS 1.0 corpus 1.1. Ljubljana: Jožef Stefan Institute, 2021. CLARIN.SI data & tools. http://hdl.handle.net/11356/1365. [COBISS.SI-ID 53371907]

13. Taherizadeh, Salman, Apostolou, Dimitris, Verginadis, Yiannis, Grobelnik, Marko, Mentzas, Gregoris. A semantic model for interchangeable microservices in cloud continuum computing. Information. 2021, vol. 12, no. 1, 40-1-40-22. ISSN 2078-2489. DOI: 10.3390/info12010040. [COBISS.SI-ID 47750147], [SNIP, WoS until 20 January 2022: total citations (TC): 2, citation index (CI): 2, citation index per author (CIAu): 0.40, Scopus until 27 January 2022: total citations (TC): 2, citation index (CI): 2, citation index per author (CIAu): 0.40]

Organization of Conferences, Congresses and Meetings

1. Launch event of IRCAI, 29 – 30 March 2021 (online)
2. SiKDD, Slovenian KDD Conference, Ljubljana, 4 October 2021
3. We ran a series of events, panels and round tables, (online) on different themes within artificial intelligence in cooperation with the Ministry of Foreign Affairs and Slovenian embassies abroad (Canada, UK, Germany, UAE, Israel, Switzerland, Romania, Japan, France) (online)
4. Digital Hackaton, Cankarjev Dom, Ljubljana, 9 – 11 November 2021

INTERNATIONAL PROJECTS

1. European Language Grid (GA 825627)
   Asst. Prof. Simon Krek
   Dfki Gmbh - Deutsches Forschungszentrum fuer Kuenstliche Intelligenz GmbH
2. INEA/CEF - MARCELL, Multilingual Resources for CEF.AT in the Legal Domain
   Asst. Prof. Simon Krek
   Innovation And Networks Executive Agency (inea)
3. INEA/CEF: CURLICAT; Curated Multilingual Language Resources for CEF AT
   Asst. Prof. Simon Krek
   Innovation And Networks Executive Agency (inea)
4. INEA/CEF: FedTerm; Federated eTranslaton Termbank Network
   Asst. Prof. Simon Krek
   Innovation And Networks Executive Agency (inea)
5. PPPA - ELE; European Language Equality
   Asst. Prof. Simon Krek
   European Commission
6. ERASMUS+: BRIDGES - Bridging Educational Emergency to Digital Pedagogies
   Kim Sevšek
   Agenzia Nazionale Erasmus Plus Indire
7. COST CA19209; European Network for Web-Centred Linguistic Data Science
   Asst. Prof. Simon Krek
   Cost Association Aisbl
8. COST CA18231; Multi3Generation: Multi-Task, Multilingual, Multi-Modal Language Generation
   Marko Grobelnik
   Cost Association Aisbl
9. H2020 - Water4Cities; Holistic Surface Water and Groundwater Management for Sustainable Cities
   Marko Grobelnik
   European Commission
10. H2020 - SILKNOW; Silk Heritage in the Knowledge Society; From Punched Cards to Big Data, Deep Learning and Visual/Tangible Simulations
    Prof. Dunja Mladenić
    European Commission
11. H2020 - COG-LO; COGnitive Logistics Operations through secure dynamic and ad-hoc collaborative networks
    Marko Grobelnik
    European Commission
12. H2020 - EnviroLENS; Coprenicus for Environmental Law Enforcement Support
    Marko Grobelnik
    European Commission
13. H2020 - Cleopatra; Cross-Lingual Event-Centric Open Analytics Research Academy
    Marko Grobelnik
    European Commission
14. H2020 - FIN-TECH; A FINancial supervision and TECHnology compliance training programme
    Marko Grobelnik
    European Commission
15. H2020 - NAIADES; A Holistic Water Ecosystem for Digitisation of Urban Water Sector
    Marko Grobelnik
    European Commission
16. H2020 - CyberSANE; Cyber Security Incident Handling, Warning and Response System for the European Critical Infrastructures
    Marko Grobelnik
    European Commission, the Directorate-General
17. H2020 - INFINITECH; Tailored IoT&BigData Sandboxes and Testbeds for Smart, Autonomous and Personalized Services in the European Finance and Insurance Services Ecosystem
    Marko Grobelnik
    European Commission
18. H2020 - FACTLOG; Energy-aware Factory Analytics for Precess Industries
    Prof. Dunja Mladenić
    European Commission
19. H2020 - HumanE-AI-Net; HumanE AI Network
    Marko Grobelnik
    European Commission
20. H2020 - STAR; Safe and Trusted Human Centric Artifical Intelligence in Future Manufacturing Lines
    Marko Grobelnik
    European Commission
21. H2020 - ODEUROPA: Negotiating Olfactory and Sensory Experiences in Cultural Heritage Practice and Research
    Prof. Dunja Mladenić
    European Commission
22. H2020 - EU-Japan.Ai: Advancing Collaboration and Exchange of Knowledge Between the EU and Japan for AI-Driven Innovation in Manufacturing
    Marko Grobelnik
    European Commission
23. H2020 - ATHENA; Implementing Gender Equality Plans to Unlock Research Potential of RPOs and RFOs in Europe
    Prof. Dunja Mladenić
    European Commission
24. H2020 - ELEXIS; European Lexicographic Infrastructure
    Asst. Prof. Simon Krek
    European Commission

RESEARCH PROGRAMME

1. Knowledge Technologies
   Prof. Dunja Mladenić

R&D GRANTS AND CONTRACTS

1. New modes and Global Patterns of Online News (Re)production
   Prof. Dunja Mladenić
2. Correlating desired phenotypic traits using behavioural, physiological and anatomical features with genetic markers in Lipizzan horse
   Dr. Aljaž Košmerlj
3. Causalify - Causality in global social dynamics
   Prof. Dunja Mladenić
4. Slovenian Artificial Intelligence Observatory
   Prof. Dunja Mladenić
5. For the Quality of Slovene Textbooks
   Asst. Prof. Simon Krek
   Ministry of Education, Science and Sport
6. Development of Slovene in the digital environment
   Dr. Aljaž Košmerlj
   Ministry of Culture
7. IRCAI - International Research Center for Artificial Intelligence – UNESCO
   Mitja Jermol, M. Sc.
   Ministry of Education, Science and Sport
8. Accompanying corpus and accompanying data sources, JR-infrastructure-SJ-2021-2022
   Dr. Iztok Kosem
   Ministry of Culture
9. Financing of projects visits at the Slovenian higher education institutions
   Dr. Alenka Guček
   Public Scholarship, Development, Disability and Maintenance Fund of the Republic of Slovenia
10. Slovenian Artificial Intelligence Observatory
    Prof. Dunja Mladenić
    Ministry of Public Administration
11. Slovenian Artificial Intelligence Observatory
    Prof. Dunja Mladenić
    Ministry of Economic Development and Technology
12. Slovenian Artificial Intelligence Observatory
    Prof. Dunja Mladenić
    Ministry of Foreign Affairs
13. Slovenian Artificial Intelligence Observatory
    Prof. Dunja Mladenić
    Government Office for the Protection of Classified Information
14. Preparation and Analysis of Data for Workshops
    Dr. Iztok Kosem
    Universidade de Coimbra
15. A Series of Events Organized with the Slovenian Embassies
    Mihajela Črnko
16. Management of the European Statistics Award for Web Intelligence - LOT 1
    Marko Grobelnik
    European Commission
17. Management of the European Statistics Award for Nowcasting - LOT 2
    Marko Grobelnik
    European Commission

VISITORS FROM ABROAD

1. Ueli Maurer, Federal Councillor, Switzerland, 28 May 2021
2. Dirk Lindemann, Director at the Federal Office for Information Technology and Telecommunications BIT, Switzerland, 28 May 2021
3. Ambassador Extraordinary and Plenipotentiary Denis Knobel, Embassy of Switzerland, Switzerland, 28 May 2021
4. Alexandra Baumann, diplomatic adviser, Federal Councillor of Finance, Switzerland, 28 May 2021
5. Marjana Tišler, Embassy of Switzerland, Switzerland, 28 May 2021
6. Manja J.Č. Vesel, protocol of the Slovenian Ministry of Finance, Switzerland, 28 May 2021
7. Veronika Novak, assistant to Ambassador Extraordinary and Plenipotentiary, Embassy of Switzerland, Switzerland, 28 May 2021
8. Jabralah Alsolami Mohammed, delegation of Saudi Arabia, Saudi Arabia, 2 September 2021
9. Amal Badr Haraka, delegation of Saudi Arabia, Saudi Arabia, 2 September 2021
10. Peter Hanke, Executive City Councillor of Finance, Business, Labour, International Affairs and Vienna Public Utilities, Vienna, Austria, 6 September 2021
11. Philipp Kamper, office of the Executive City Councillor of Finance, Business, Labour, International Affairs and Vienna Public Utilities, Vienna, Austria, 6 September 2021
12. Martin Ritzmaier, office of the executive City Councillor of Finance, Business, Labour, International Affairs and Vienna Public Utilities, Vienna, Austria, 6 September 2021
13. Oliver-John Perry, Media spokesman for City Councillor for Finance, Labour, Economy, International Affairs and Wiener Stadtwerke, Vienna, Austria, 6 September 2021
14. Markus Pöllhuber, director WH Digital GmbH (Eurocomm-PR), Vienna, Austria, 6 September 2021
15. Sanja Dražić, procurator WH Digital GmbH (Eurocomm-PR), Vienna, Austria, 6 September 2021
16. Daniela Bichiou, Business Relation Manager EU (Eurocomm-PR), Vienna, Austria, 6 September 2021
17. Saša Ljubec, Head of the Vienna Representation in Ljubljana (Eurocomm-PR), Vienna, Austria, 6 September 2021
18. Jana Veber, interpreter for German language, Vienna, Austria, 6 September 2021
19. Žiga Intihar, photographer, Vienna, Austria, 6 September 2021
20. Florian Sekira, ORF Journalist, Vienna, Austria, 6 September 2021
21. Stefanie Rachbauer, Editor at KURIER, Vienna, Austria, 6 September 2021
22. Gerald Mackinger, journalist at Austria Press Agency, Vienna, Austria, 6 September 2021
23. Christian Nusser, journalist at Heute, Vienna, Austria, 6 September 2021
24. Thomas Cervenka, chauffeur to Federal Councillor, Vienna, Austria, 6 September 2021
25. Kilian Gross, European Commission, Brussels, Belgium, 15 September 2021
26. Dejan Dvoršek, European Commission, Brussels, Belgium, 15 September 2021
27. Mark Boris Andrijanič, Minister of Digital Transformation, Ljubljana, Slovenia, 15 September 2021
28. Samo Zorc, Ministry of Public Administration, Ljubljana, Slovenia, 15 September 2021
29. Polonca Blaznik, Ministry of Public Administration, Ljubljana, Slovenia, 15 September 2021
30. Igor Zorko, Chambers of Commerce, Association for Informatics and Telecommunications (ZIT), Ljubljana, Slovenia, 15 September 2021
31. Ken Kitatani, director, I-CEED, 20 - 21 September 2021
32. Kazunao Sato, executive director, I-CEED, 20 - 21 September 2021
33. Georges Rebelo Chikoti, Secretary General of the Organization of African, Caribbean and Pacific States, Brussels, Belgium, 28 September 2021
34. John F. Kakule, ACP Secretariat, Brussels, Belgium, 28 September 2021
35. Agim Kukaj, director of ICT department, Ministry of Economy, Pristina, Kosovo, 28 September 2021
36. Sara Ibrahimi, Ministry of Economy, Pristina, Kosovo, 28 September 2021
37. Adnan Ahmeti, Office of the Prime Minister, Pristina, Kosovo, 28 September 2021
38. Venhar Nushi, Office of the Prime Minister, Pristina, Kosovo, 28 September 2021
39. Vesna Prodnik, CEO at VAFER Ltd, Pristina, Kosovo, 28 September 2021
40. Coletté Mélot, Senator of France, France, 29 September 2021
41. Nicole Duranton, Senator of France, France, 29 September 2021
42. Jean Bonhomme, Senator of France, France, 29 September 2021
43. Elena Richard, chancellerie poltique, Embassy of France, France, 29 September 2021
44. Valentine Morel, attaché for scientific cooperation, France, 29 September 2021
45. Akmal Burkhanov, Director of the Anti-Corruption Agency of Uzbekistan (ACA), Uzbekistan, 15 October 2021
46. Sukhrob Alimukhamedov, Representative of the President Administration, Uzbekistan, 15 October 2021
47. Abror Yadgarov, Lead inspector of Internal security division, Uzbekistan, 15 October 2021
48. Akbar Ergashev, Director's advisor, Uzbekistan, 15 October 2021
49. Kobil Khidirov, Member of ACA Public Council (journalist), Uzbekistan, 15 October 2021
50. Ulugbek Daulanov, Deputy Head of the Anti-corruption system monitoring and analysis department, Uzbekistan, 15 October 2021
51. Nodirbek Ashurov, Lead inspector of the State officials' assets and income declaration department, Uzbekistan, 15 October 2021
52. Darya Zemeseva, Regional Dialogue Branch Office in Uzbekistan (interpreter), Uzbekistan, 15 October 2021
53. Nodirjon Juraev, Regional Dialogue Branch Office in Uzbekistan, Uzbekistan, 15 October 2021
54. Jack Roger Anderson, Representative of U.S. Embassy in Tashkent, Director of INL in Uzbekistan, Uzbekistan, 15 October 2021
55. Azizbek Yusupov, Representative of U.S. Embassy in Tashkent, INL Program Specialist in Uzbekistan, Uzbekistan, 15 October 2021
56. Furkat Kayumkhodjayev, Representative of U.S. Embassy in Tashkent, INL Program Assistant in Uzbekistan, Uzbekistan, 15 October 2021
57. Petra Gorjup, Head of Branch Office of Regional Dialogue, Logatec, Slovenia, 15 October 2021
58. Mjuša Sever, Director of Regional Dialogue, Logatec, Slovenia, 15 October 2021
59. Dobran Božič, Deputy Head of the Government Office for the Protection of Classified Information, Ljubljana, Slovenia, 15 October 2021
60. Katja Geršak, Head of CEP-Center for European Perspective, Ljubljana, Slovenia, 15 October 2021
61. Signe Riemer-Sørensen, Sintef, Trondheim, Norway, 7 - 10 November 2021
62. Till Christopher Lech, Sintef, Trondheim, Norway, 7 - 10 November 2021
63. Lene Lad Johansen, Sintef, Trondheim, Norway, 7 - 10 November 2021

STAFF

Researchers
1. Asst. Prof. Branko Kavšek*
2. Dr. Iztok Kosem
3. Asst. Prof. Simon Krek
4. Dr. Jurij Leskovec
5. **Prof. Dunja Mladenić**, Head
6. Prof. John Stewart Shawe-Taylor
7. Asst. Prof. Primož Škraba

Postdoctoral associates
8. Dr. Luka Bradeško
9. Dr. Kaja Dobrovoljc
10. Dr. Blaž Fortuna*
11. Dr. Alenka Guček
12. Dr. Aljaž Košmerlj
13. Dr. David Lindemann
14. *Dr. Joao Paulo Pita Da Costa*, left 01.06.21*
15. Dr. Adam Rambousek
16. Dr. Jan Rupnik*
17. *Ayse Saliha Sunar, B. Sc., left 01.06.21*

Postgraduates
18. Swati , M. Sc.
19. Jaka Čibej, B. Sc.
20. Rayid Ghani, M. Sc.
21. James Alexander Hodson, B. Sc.
22. Jakob Jelenčič, B. Sc.
23. Mitja Jermol, M. Sc.

24. Klemen Kenda, B. Sc.
25. Mark D Minevich, M. Sc.
26. Erik Novak, B. Sc.
27. *Eva Pori, B. Sc., left 01.04.21*
28. Jose Martin Rožanec, M. Sc.
29. Abdul Sittar, M. Sc.

Technical officers
30. Dr. Janez Brank
31. Dr. Miha Cimperman
32. Teja Goli, B. Sc.
33. Dr. Matej Kovačič
34. Dr. Gregor Leban*
35. Jose Luis Machado Rei, M. Sc.
36. Dr. Inna Novalija
37. Dr. Ervin Pfeifer*
38. Primož Ponikvar, B. Sc.
39. Matej Posinković, B. Sc.
40. Dr. Polona Škraba Stanič
41. Maja Škrjanc, B. Sc.

Technical and administrative staff
42. Aleš Buh
43. Mihajela Črnko
44. Jasna Franko, B. Sc.
45. Marko Grobelnik
46. *Blaž Kažič, B. Sc., left 01.09.21*
47. Mojca Kregar, B. Sc.

48. Monika Kropej, B. Sc.
49. *Tina Munda, B. Sc., left 01.10.21*
50. Blaž Novak, B. Sc.
51. *Davor Orlić, B. Sc., left 01.12.21*
52. Kim Sevšek, B. Sc.

53. Špela Sitar, B. Sc.
54. Mateja Škraba, B. Sc.

Note:
* part-time JSI member

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THESES AND MENTORING

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LABORATORY FOR OPEN SYSTEMS AND NETWORKS E-5

The main activities of the laboratory are R&D in the area of next-generation networks, telecommunications technologies, components and integrated systems, information-society services, mechanisms and applications, especially those that enable better privacy protection of citizens and an increased trustworthiness of information and communication technologies and services.

The research in 2021 was performed within the research programme *Future Internet Technologies: concepts, architectures, services and socio-economic issues*, funded by the Slovenian Research Agency. In addition, research was carried out within the EU Horizon 2020 projects *CONCORDIA*, *DE4A*, *BD4OPEM* and *iFlex*, the EU DG Justice *EIO-LAPD* project, the *SI-PASS 2.0* project from the CEF programme, national projects *Artificial intelligence for cybersecurity* and *Evaluation of IP as a basis for proposing a long-term sustainable state aid model to promote science-business cooperation*, and an industrial project called *Use Wisely* with Elektro Celje. The focus was on the development of the technologies and services within advanced next-generation networks, security and privacy in information systems, and technology-enhanced learning.

Members of the laboratory teach at the undergraduate and graduate levels at the Jožef Stefan International Postgraduate School, the DOBA Faculty, and the Faculty of Commercial and Business Sciences. The laboratory is a member of the European Cyber Security Organisation (ECSO).

Head:
Asst. Prof. Tomaž Klobučar

Concepts and architectures of the secure internet, internet technologies and information systems

The first area of research and development included security infrastructures and secure services as well as internet technologies in the energy and e-health domains.

The main goal of the *SI-PASS 2.0* (Integrating Slovenian e-services with the national eIDAS node) project from the EU CEF (Connecting Europe Facility) programme was to set up secure cross-border services, based on national electronic identification means, in different application domains. The *SI-PASS 2.0* project, which was coordinated by the Laboratory for Open Systems and Networks, integrated five public and one private cross-border e-services with the Slovenian national eIDAS node in the fields of e-government, higher education, municipalities, health insurance and financial services. The eIDAS node is the central point of trust in the country, set up at the Ministry of Public Administration according to the EU eIDAS regulation (The regulation on electronic identification and trust services for electronic transactions in the internal market) requirements. On the one hand, it connects national infrastructure with international service providers and, on the other hand, the national identity and service providers with the infrastructures of the other EU countries. The results of the project enable citizens of EU Member States to access Slovenian e-services with their national notified electronic identification means.

> **We have created building blocks for security infrastructures and secure internet services.**

Similar objectives are pursued by the three-year **DE4A** (*Digital Europe for All*) project that aims at facilitating migration towards secure European digital public services, co-delivered across borders, across sectors and with different participants, and at implementing the latest EU directives and regulations (e.g., eIDAS, Single Digital Gateway). The project simplifies the cross-border user interaction with the selected procedures, systems and platforms, and demonstrates, in practice, the benefits of realizing cross-border principles of Once-Only and Digital-by-Default for different stakeholders. Our main role in the project is to coordinate the *Studying Abroad* pilot, one of the three project pilots, and carry out an analysis of the current eGovernment landscape. The pilot implements and validates the cross-border higher-education procedures of the Single Digital Gateway Regulation, in particular the applications to higher-education institutions, applications for study grants, and recognition of diplomas. In 2021 we developed and set up a grant application service that allows students from Portugal and Spain to use their national eIDs to access the services and explicitly request the use of the DE4A technical system to have their diploma evidence required by the service transferred electronically from a trusted source in their home country. In this way, students no longer have to search for the evidence and fill in the necessary application forms by themselves.

Figure 1: Infrastructure for secure cross-border services

Other Slovenian partners in the project launched in 2020 are the Ministry of Education, Science and Sport, the Ministry of Public Administration, and the University of Maribor.

The **BD4OPEM** (*Big Data for Open Innovation Energy Marketplace*) project uses a data-centric approach to innovate between the needs of energy stakeholders and the solutions being developed. A data flow through the marketplace enables the development of analytic services to boost business processes. To date, the laboratory has focused on predictive maintenance, non-technical loss analysis, flexibility prediction in the distribution network, and privacy and security of the marketplace and services. An anonymisation service for time-series data was developed. Two JSI departments, our laboratory and the Department of Communication Systems, participate in the project, while the key Slovenian partner from the energy sector is Elektro Celje.

Figure 2: Detection of non-technical losses

Internet technologies facilitate integration of end-users in the electricity market and help power distributors in the market operation.

The **iFlex** (*Intelligent Assistants for Flexibility Management*) project focuses on the design, development and evaluation of supporting tools for effective consumer participation in various flexibility services of the smart grid of the future and for their easier pursuit of sustainability goals in their premises. A strong Slovenian consortium is participating in the project: Elektro Celje, Elektro Celje Energija, Smart Com, Slovene Consumers Associations and JSI, Laboratory for Open Systems and Networks. The tasks of the laboratory include the security and privacy of the project solution, data analytics, consumer profiling, development of the digital twin of the consumer premises and optimal multicriteria control of the consumer home power consumption.

The **Use wisely** project evaluated flexibility services in a distribution network. The laboratory project work focused on data analytics, peak forecasting, consumer response assessment, and cloud services support. As part of the project, we evaluated the end-user response to positive tariffs and their ability to lower critical peaks as well as the response to negative tariffs and end-user ability to consume more energy during a surplus of the photovoltaic generation. In 2021 a large-scale piloting of positive and negative critical peak tariffs with more than 800 consumers was conducted in the Celje region. During the pilot, 41 flexibility events were forecasted, planned and analysed for Elektro Celje. Other partners in the project, funded by the Energy Agency, include Elektro Celje, Smart Com and Comsensus. The agency also approved grants for the use of positive and negative tariffs in 2021.

Figure 3: Assessment of end-user flexibility in smart grids

As part of the **infrastructure programme in research organizations**, we continue to provide support services that enable better communication among members of various research programs as well as students and their mentors from geographically dispersed institutions. These services proved crucial to the smooth operation of the Institute during the COVID-19 pandemic. In addition, the infrastructure programme provided 20 GoToMeeting licences and, together with the Centre for Network Infrastructure, additional 100 Zoom licences. The licences were provided to 31 departments, laboratories, centres and other organizational units of the Institute. With the help of the research-infrastructure services, more than 6085 meetings were held at the JSI in 2021 with 48,500 participants for a total of 46,000 hours (1916 days). We also supported the organization and implementation of the Slovenian and European Science Festival 2021.

Mechanisms for security and privacy provision in information systems

Ensuring the security and privacy of information systems is key to the functioning of the modern information society and the development of an efficient digital market. A major research challenge for ensuring system and service security is the prevention of cybercrime. In 2021 the researchers of the Laboratory worked intensely on developing solutions and systems for the provision of the necessary security mechanisms.

In this context, our method and software tool were improved to identify the vulnerable internet systems on the global internet, which can scan almost all available WordPress-based web servers on the internet. Measures and mechanisms were proposed to address the identified vulnerabilities. A key feature of the developed method and tool, named Vulnet, is its ability to automatically, quickly, and dynamically identify vulnerabilities on a large scale, while also considering the ethical aspects of the investigated web servers. The research resulted in the best paper award at the INTERNET 2021 conference. The tool is now available as a free-of-charge service for the web owners for checking and preventing the vulnerabilities of their web sites.

Another research topic was mathematical models for constructing significant Boolean functions used in symmetric cryptographic algorithms. We studied a class of p-ary functions $f_{(\lambda,u,v)}(x)=Tr_1^k(\lambda x^{p^k+1})+Tr_1^n(ux)Tr_1^n(vx)$ for any odd prime p. Using Fourier transforms, we were able to subdivide the class of all $f_{(\lambda,u,v)}$ into subclasses of bent, near-bent and 2-plateaued functions. This classification is important because the subclass functions have various desirable cryptographic properties (they can be balanced for both an odd and even number of variables, and they do not possess nonzero linear structures) and play a significant role in certain cryptographic primitives. The results were published in the scientific journal AIMS Mathematics. Another important result was a study of an open problem regarding the EA-inequivalence among the classes of bent functions. We utilized second-order derivatives as invari-

ants to determine, at least partially, the EA-inequivalence of the bent functions with the same algebraic degree. This method provided the necessary and sufficient conditions for establishing the EA-equivalence between certain cubic bent functions of the Mairona-McFarland class. The results were published in a scientific journal entitled Applicable Algebra in Engineering, Communication and Computing.

The infrastructure programme services proved crucial to the smooth operation of the Institute during the COVID-19 pandemic.

In 2021 we also had our research on privacy threats and countermeasure in online social networks published in a book chapter. Solove's taxonomy of privacy violations has been refined to incorporate modern challenges into the privacy posed by the evolution of social networks. This work emphasizes the fact that privacy protection should be a joint effort of social network owners and users, and provides a classification of mitigation strategies according to the party responsible for taking these countermeasures. In addition, it highlights the key research issues to guide the research in the field of privacy preservation.

Advanced technologies that promise a more effective cybersecurity provision include artificial intelligence (AI), which is especially useful in analysing and processing a large number of security-relevant events and in detecting and responding to unknown threats and forms of cyber attacks. In addition to appropriate competences and joint collaboration, information on research gaps in this field and R&D capabilities as well as the comparative advantages of Slovenia are also important for more efficient research and development and the breakthrough of Slovenian security solution providers on the EU and global markets. The *Artificial intelligence for cybersecurity* project is aimed at research of the AI methods, use cases of cybersecurity, analysing the current situation in this field in Slovenia, EU and the rest of the World, identifying potential areas where Slovenia has comparative advantages and development potential, and preparing the guidelines proposals for the development. In 2021 we developed the taxonomy of the use of AI for cybersecurity provision and prepared a systematic literature review on this topic that will serve as the basis for the research gap analysis.

Research on the acquisition of cross-border digital evidence in crime investigation, enabled by the implementation of Directive 2014/41/EU and Slovenian legislation, was part of the *EIO-LAPD* (European Investigation Order – legal analysis and practical dilemmas of international cooperation) project funded by the EU DG Justice. The project is based on the cooperation of the institutions from Austria, Croatia, Italy, Germany and Portugal. The last year of the project was focused on dissemination of the research results on the legal instruments for cross-border crime investigation through conference presentations and professional articles.

The Laboratory for Open Systems and Networks is a member of **CONCORDIA** (Cyber security competence for research and innovation), one of the four European centres of excellence in cyber security from the H2020 programme with leading competences in research, technology, industry and the public domain. The centre provides research and development solutions for a safe, resilient and trustworthy European ecosystem. Within CONCORDIA, the laboratory

Our research and development results enable a more secure information society.

contributes the research on user-centric security, mainly through models for fighting disinformation, facilitating online trust management and establishing electronic identities. In addition, the laboratory is actively involved in the e-Health pilot, also contributing the data and models for developing threat intelligence models as well as cybersecurity education activities. In 2021 the Laboratory participated in a large survey among the EU high-school teachers, students and parents with the aim to provide the content and delivery methods for sustainable cybersecurity education. An overview of the games to be used in the cybersecurity education was prepared. The survey results reveal important issues and allow appropriate recommendations to be made. As a result of this work, two articles were published in journals with a high impact factor.

Information society services, applications and socio-economic issues

The development of the digital market is conditioned by the development of appropriate information services, such as technologically supported teaching and the raising of the level of digital skills, and improvement of the quality of life of older adults. Our research was focused on assisting older adults to acquire digital skills when they have little or no prior experience with technology use. To facilitate learning we introduced a gamified environment

and peer-to-peer interaction along with a digital mentor. We established verbal and non-verbal communication patterns that support learning and cooperative action between paired participants. We also examined the efficacy of a minimalist approach in mentoring. Our research with older adults expanded with a study that evaluated different approaches in using smartphone sensors to capture spatial and temporal variables for mobility tests. We proved the validity and reliability of the approach for the sit-to-stand test as we commenced with research into other evaluation models for different mobility tests.
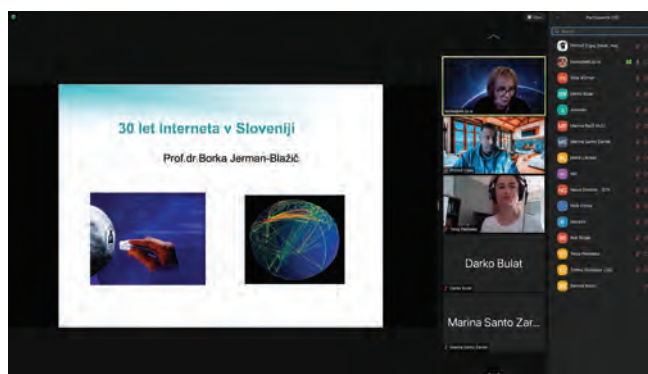
Figure 4: 30th anniversary of the first internet connection in Slovenia

In 2021 we initiated research into the use of mobile image processing in tracking and assessing wound severity. Initially, we performed a systematic investigation of the research to determine the current image-processing techniques used in wound estimation where we discovered that the most dominant image-processing colour model was HSV and that the mobile technology reached the level or reliable accuracy. Next, we devised a method for using mobile-image processing in the measurement the wound area, and we implemented the method within the OpenCV framework. Our approach relies on a multi-step process consisting of image capture, conversion to grayscale, blurring, application of a threshold with segmentation, identification of the wound part, dilation and erosion of the detected wound section, identification of the accurate data related to the image, and measurement of the wound area. This is a potential solution that can be used in healthcare systems to investigate and treat people with skin-related diseases.

The Laboratory for Open Systems and Network is involved with several other research departments and Director's Office at the Jožef Stefan Institute within the *Athena* project aiming at removing barriers to the recruitment, retention and career progression of female researchers, lowering gender imbalances in decision-making processes and generating a cultural change needed to avoid gender bias and discriminatory practices through the implementation of Gender Equality Plans (GEPs). To ensure a systemic institutional change, the project plans to assess procedures and practices already in place in partner organizations, together with an analysis of the national legislation and policy frameworks. In parallel, it will put in place a participatory process aimed, on the one hand, to understand the needs and preferences of the stakeholders and, on the other hand, to train them about the selected topics related to gender. As a final result, each partner organization will draft and implement its specific GEP. In 2021 the Laboratory for Open Systems and Networks contributed an analysis of the answers to the survey about the attitudes of the JSI employees towards different aspects of the gender equality at their organization to the document *Implementing gender equality plans to unlock research potential of RPOs and RFOs in Europe.*

Prof. Dr. Borka Jerman Blažič received the Puh Award for Life Achievements in the field of information and communication technologies.

In 2021 in collaboration with the Centre for Technology Transfer and Innovation at the Jožef Stefan Institute, we started a new national project on the evaluation of intellectual property as the basis for proposing a long-term sustainable state aid model to promote the science-business cooperation. The project, funded by the Ministry of Education, Science and Sport and the Slovenian Research Agency, will quantitatively and qualitatively analyse the critical points of intellectual property rights (IPR) transfer and prepare guidelines for the IPR management in collaborative R&D projects. An international comparative review of the regulation of state aid systems, a proposal for a sustainable state aid system and the changes that should be implemented in order to achieve a more effective cooperation in the innovation helix will also be prepared.

The Laboratory is also an active member of the IEEE P2933 Working Group on Clinical IoT standardisation. It co-chairs the Trust and Identity Subgroup (T&I SG) and is an active member of the Artificial Intelligence & Machine Learning SG and the Intelligent System Design SG. As part of the standard, the Laboratory is leading the standard development methodology from and Identity and Trust aspect, the taxonomy of the Clinical IoT system design and the alignment between the different sub-groups in the integration of their parts into the standard's architecture. At the same time, the Laboratory is acting as a link between the EU and US (technological and regulatory) perspectives on trust and identity in Clinical IoT, bringing into the standard the experience and lessons learned from the e-SENS and CONCORDIA architectures for the e-health pilots. In 2021 we were involved in the drafting of the Trust and Identity part of the standard, covering the parts on: computational trust model for Clinical IoT architecture, inter-dependence between trust and identity, and integration of trust and identity into the Clinical IoT reference architecture.

Figure 5: Puh Award for Life Achievements for Prof. Borka Jerman Blažič

Science promotion and awards

In November we celebrated the 30th anniversary of the first international internet connection in Slovenia that was established in 1991 in the Laboratory for Open Systems and Networks. The connection was a result of the *EUREKA-8/COSINE* (Cooperation of Open Systems Interconnections) project, in which the Laboratory was involved. As part of the online celebration event, Nick Hyrik from the International Internet Society (ISOC) addressed the audience, while members of the laboratory gave several lectures. Prof. dr. Borka Jerman Blažič presented the beginnings of the internet in Slovenia, dr. Primož Cigoj presented a tool for a more efficient detection of vulnerable sites, while Tanja Pavleska discussed cyber security and disinformation in Europe and Slovenia. The President of the Republic of Slovenia paid tribute to the anniversary with a reception at the Presidential Palace.

Among the received prizes in 2021, we highlight the Puh Award for Life Achievements, which was received by prof. dr. Borka Jerman Blažič for her contributions to the field of information and communication technologies.

Some outstanding publications in the past three years

1. Jerman-Blažič, Borka. The cybersecurity labour shortage in Europe: moving to a new concept for education and training. Technology in Society, ISSN 0160-791X. [Print ed.], 2021, vol. 67, pp. 101769-1-101769-13.
2. Luís Marques, Diogo, Pereira Neiva, Henrique, Miguel Pires, Ivan, Zdravevski, Eftim, Mihajlov, Martin, Garcia, Nuno M., Ruiz-Cárdenas, Juan Diego, Almeida Marinho, Daniel, Cardoso Marques, Mário. An experimental study on the validity and reliability of a smartphone application to acquire temporal variables during the single sit-to-stand test with older adults. Sensors, ISSN 1424-8220, 2021, vol. 21, pp. 2050-1- 2050-15.

Organization of conferences, congresses and meetings

1. 27th Slovenian Festival of Science with international participants, 28–30 September 2021, (virtual).
2. European Festival of Science, 9-11 November 2021, (virtual).
3. 30th anniversary of the Internet in Slovenia: Celebration of the first Internet connection at the Jožef Stefan Institute, 24 November 2021, (virtual).

INTERNATIONAL PROJECTS

1. EIO-LAPD-JUST-AG-2018/JUST-JCOO-AG-2018; European Investigation Order - Legal Analysis and Practical Dilemmas of International Cooperation
   Prof. Borka Džonova Jerman Blažič
   European Commission, Directorate General Justice
2. ERASMUS+; DigiBlend - Improving Adult Digital Literacy Through Innovative Gamified Blended Learning
   Dr. Martin Mihajlov
   European Commission
3. INEA/CEF - SI-PASS 2.0.; Integrating Slovenian E-Services with the National eIDAS Node
   Asst. Prof. Tomaž Klobučar
   European Commission
4. H2020 - CONCORDIA; Cyber Security Competence Research and Innovation for Research and Innovation
   Dr. Tanja Pavleska
   European Commission
5. H2020 - DE4A; Digital Europe for All
   Asst. Prof. Tomaž Klobučar
   European Commission
6. H2020 - BD4OPEM; Big Data for Open Innovation Energy Marketplace
   Dr. Dušan Gabrijelčič
   European Commission
7. H2020 - iFLEX; Intelligent Assistants for Flexibility Management
   Dr. Dušan Gabrijelčič
   European Commission
8. H2020 - ATHENA; Implementing Gender Equality Plans to Unlock Research Potential of RPOs and RFOs in Europe

Prof. Borka Džonova Jerman Blažič
European Commission

RESEARCH PROGRAMME

1. Future Internet Technologies: concepts, architectures, services and socio-economic issues
   Prof. Borka Džonova Jerman Blažič

R&D GRANTS AND CONTRACTS

1. Artificial intelligence for cybersecurity
   Asst. Prof. Tomaž Klobučar
2. Evaluation of IP as a basis for proposing a long-term sustainable state aid model to promote science-business cooperation
   Prof. Borka Džonova Jerman Blažič
3. Artificial intelligence for cybersecurity
   Asst. Prof. Tomaž Klobučar
   Government Information Security Office

NEW CONTRACT

1. "Use Wisely" project support
   Dr. Dušan Gabrijelčič
   Elektro Celje d. d.

STAFF

Researchers
1. Asst. Prof. Rok Bojanc*
2. Prof. Borka Džonova Jerman Blažič
3. Dr. Dušan Gabrijelčič
4. **Asst. Prof. Tomaž Klobučar, Head**
5. Dr. Martin Mihajlov
Postdoctoral associates
6. Dr. Ramanpreet Kaur
7. Dr. Samed Bajrić
8. Dr. Andrej Jerman Blažič
9. Dr. Tanja Pavleska

10. Dr. Živa Stepančič
Postgraduate
11. Dr. Primož Cigoj
Technical officer
12. Klemen Stanič, B. Sc.
Technical and administrative staff
13. Tatjana Martun, B. Sc.

Note:
* part-time JSI member

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3. Diogo Luís Marques, Henrique Pereira Neiva, Ivan Miguel Pires, Eftim Zdravevski, Martin Mihajlov, Nuno M. Garcia, Juan Diego Ruiz-Cárdenas, Daniel Almeida Marinho, Mário Cardoso Marques, "An experimental study on the validity and reliability of a smartphone application to acquire temporal variables during the single sit-to-stand test with older adults", *Sensors*, 2021, **21**, 6, 2050.
4. Filipe Ferreira *et al.* (11 authors), "Experimental study on wound area measurement with mobile devices", *Sensors*, 2021, **21**, 17, 5762.
5. Borka Jerman-Blažič, "The cybersecurity labour shortage in Europe: moving to a new concept for education and training", *Technology in society*, 2021, **67**, 101769.

Review Article

1. Filipe Ferreira da Salva, Ivan Miguel Pires, Monica Jones Costa, Vasco Ponciano, Nuno M. Garcia, Eftim Zdravevski, Ivan Chorbev, Martin Mihajlov, "A systematic investigation of models for color image processing in wound size estimation", *Computers*, 2021, **10**, 4, 43.

Published Conference Contribution (invited lecture)

1. Borka Jerman-Blažič, Primož Cigoj, "Web vulnerability in 2021: large scale inspection, findings, analysis and remedies", In: *Internet 2021, The Thirteenth International Conference on Evolving Internet, July 18-22 2021, Nice, France*, Proceedings, IARIA, 2021, 24-30.

Published Conference Contribution

1. Helder Aranha, Massimiliano Masi, Tanja Pavleska, Giovanni Paolo Sellitto, "Securing the metrological chain in IoT environments: an architectural framework", In: *2021 IEEE International Workshop on Metrology for industry 4.0 and IoT, Rome, Italy, June 7-9, 2021*, Proceedings, IEEE, 2021, 704-709.
2. Giovanni Paolo Sellitto, Helder Aranha, Massimiliano Masi, Tanja Pavleska, "Enabling a zero trust architecture in smart grids through a digital twin", In: *EDCC 2021 Workshops, DREAMS, DSOGRI, SERENE 2021, Munich, Germany, September 13, 2021*, Dependable computing, (Communications in computer and information science **1462**), Springer, 2021, 73-81.

3. Tomaž Klobučar, "Varne čezmejne e-storitve in načelo "samo enkrat"", In: *28. Dnevi slovenske informatike, Portorož, 19-20 oktober 2021*, Digitalizacija: uspešneje, hitreje, ceneje, Slovensko društvo Informatika, 2021, 16-22.
4. Rok Bojanc, "Analysis of research on e-invoicing in Slovenia", In: *EECME 2021, Eastern European Conference of Management and Economics, Slovenia, Ljubljana, May 28, 2021*, Sustainable development in modern knowledge society, Ljubljana School of Business, 2021, 79-87.
5. Andrej Jerman Blažič, "Cyber security and serious games in the educational process: an exploratory study of the learning and technical parameters", In: *INTED 2021, 15th International Technology, Education and Development Conference, 8-9 March, 2021*, Proceedings, IATED Academy, 2021, 3976-3982.
6. Giovanni Paolo Sellitto, Massimiliano Masi, Tanja Pavleska, Helder Aranha, "A cyber security digital twin for critical infrastructure protection: the intelligent transport system use case", In: *PoEM 2021, 14th IFIP WG 8.1 Working Conference on the practice of enterprise modeling, Riga, Latvia, November 24-26, 2021*, Proceedings, (Lecture notes in business information processing **432**), Springer, 2021, 230-244.
7. Massimiliano Masi, Tanja Pavleska, Simone Pezzoli, "A systematic approach for the definition of countermeasures in industrial IoT: an automotive case", In: *ITASEC 2021, Italian Conference on Cybersecurity 2021*, Proceedings, (CEUR workshop proceedings **2940**), CEUR-WS, 2021, 319-330.
8. Izudin Softić, Samed Bajrić, Nedžimija Demirović, Emina Hrvić, Amila Brčaninović, "An impact of spinning reserve on the number of solutions in the unit commitment problem", In: *ERK 2021, 30th International Electrotechnical and Computer Science Conference, Portorož, Slovenia, 20-21 September 2021*, Proceedings, (Zbornik Elektrotehniške in računalniške konference **30**), Slovenska sekcija IEEE, Fakulteta za elektrotehniko, 2021, 234-237.

Independent Component Part or a Chapter in a Monograph

1. Borka Jerman-Blažič, "Cybersecurity skills in EU", In: *Cybersecurity threats with new perspectives*, IntechOpen, 2021, 190-212.
2. Ramanpreet Kaur, Tomaž Klobučar, Dušan Gabrijelčič, "Privacy in online social networks: threat analysis and countermeasures", In: *Handbook of research on cyber crime and information privacy*, IGI Global, 2021, 567-598.
3. Rok Bojanc, "Analysis of e-invoicing as a driver for digital transformation", In: *Sustainable development in a modern knowledge society*, Ljubljana School of Business, 2021, 65-76.

Theses and Mentoring

1. Primož Cigoj, *An automated vulnerability detection for website security:* doctoral dissertation, Ljubljana, 2021 (mentor Borka Jerman Blažič).

DEPARTMENT OF COMMUNICATION SYSTEMS

E-6

The core activities of the Department of Communication Systems comprise the research, development and design of heterogeneous communication, computer and sensor networks, wireless technologies and next-generation communication services; the design of new procedures for parallel and distributed computing of computationally intense problems in various high-performance computing architectures and time-sensitive problems in edge devices; and the integration of sensor, communication, computing and data technologies to support digitalization and smart infrastructures. Within these activities our research work includes the development and investigation of new methods and architectures, software tools and libraries, pilot deployments and experimental testbeds.

Head:
Prof. Mihael Mohorčič

The research and development activities at the department are carried out in three laboratories: the *Communication Technology Laboratory (CTL),* the *Parallel and Distributed Systems Laboratory (PDSL)* and the *Networked Embedded Systems Laboratory (NESL).* The research work of the three laboratories is complementary, which is reflected in the joint applied projects.

In the **Communication Technology Laboratory** we have focused mainly on the research associated with the access-segment of radio technologies. We have studied radio transmission in terrestrial and satellite communications and radio and network resource management. The research is part of the Communications Networks and Services research programme (P2-0016) and research projects J2-2507 "Towards the environment-aware intelligent wireless communications" and J2-3048 "Advanced modelling of radio channels using ray-optical and numerical meshless methods". In addition, we have continued our research in the field of power grids that we started in previous years and we have extended the LOG -a- TEC testbed with new functionalities.

An important part of the activities of the Communications Technology Laboratory has been research in radio-channel modelling and simulation. In this context, we have further investigated deterministic channel modelling, in particular ray-tracing algorithms, in irregular environments and explored new approaches and algorithms as well as environment simplification to make radiowave-propagation prediction more time-efficient and accurate.

The focus has been on investigating the performance of ray-tracing techniques in highly irregular environments consisting of many small triangular surfaces, typically obtained by laser scanning. We have studied the simplification of the environment description for the purpose of channel modelling and shown that the choice of simplification algorithm affects the degree of acceptable simplification. The approaches were tested on 3D

> **By using the radio environment fingerprint of the mobile phone, we assess the contact intensity between people.**

natural cave models and on a ray-tracing radio-propagation prediction approach. The larger tunnel-like caves show minimal accuracy changes up to the point where the cave becomes impassable, the narrower and less uniform caves show some accuracy improvements. The main advantage of the proposed approach is the reduction in modelling time, which is approximately halved for the available scan resolution. According to the results, the edge-removal simplification approach showed the best performance.

Deterministic ray-tracing techniques model only a subset of well-known radio-wave propagation mechanisms and in their present form do not provide adequate radio channel modelling for next-generation communications. Massive multiple and distributed antenna systems, the ever-increasing number of access points and the reduction of wireless cell's effective geographic area, combined with the increase in the computational power, have opened new research opportunities. Among them, the use of numerical solvers based on Maxwell's equations of electricity and magnetism is becoming more and more feasible for electrically larger problems. We have been investigating such techniques for the telecommunication channel modelling of complex environments in project J2-3048 "Advanced modelling of radio channels using ray-optical and numerical meshless methods". The acceleration of computationally demanding techniques for their greater acceptability is an alternative to accuracy improvements

Figure 1: System for measuring and displaying the angle of arrival of a signal transmitted by a BLE device.

in existing deterministic models, where in the last decade ray tracing shows a prevailing trend to replace empirical models. We have proposed a comprehensive evaluation and adaptation of the two competing approaches for the telecommunication-channel modelling. The objective of our research is to study ways of overcoming excessive time requirements while providing acceptable channel-modelling accuracy. Our focus is primarily on environments with no simple geometrical description, such as detail-rich small radio cells.

As part of the research activities in wireless-network optimization and management, we have investigated a novel method that enables the prediction of radio-channel characteristics beyond what is currently available by taking advantage of environmental information, measured partial channel state information (CSI), and information about the radio nodes applicable in future intelligent radio networks. This research is the topic of project J2-2507, "Towards the environment-aware intelligent wireless communications". The intelligence of future wireless-communication systems relies on radio environment awareness, which is estimated from the received signal properties, current and past exploited network resources. In 2021 we analysed the wireless communications in use and their ability to estimate the environment and proposed the system architecture for the proposed methodology. In addition we further explored the idea of estimating the 3D environmental geometry and electrical properties of the building elements by exploiting the channel state information and assuming an infinite frequency bandwidth for the communication system. The idea assumes that the received radio signal is distorted by the interaction with the surrounding objects and thus contains the signature of the radio environment. We proposed a novel method of using the radio environment signatures to characterize the geometry, building material, and room size by using machine-learning tools, ray-tracing simulations, and an ultra-wideband (UWB) communication technology. Computer simulations have revealed that wall materials with different electromagnetic properties and room sizes can be classified into representative groups that observe a single transmission link in the known surrounding geometry. When the geometry of the environment is not known, more than one radio link must be included in the learning and testing process. To test the hypothesis in the real environment, a handheld tool based on UWB radio technology was developed to estimate channel state information.

Figure 2: A comparison between flow cases through a porous channel that shows the difference caused by inertial effects at higher Reynolds numbers (left two plots). Relation between participation number π and Reynolds number for two randomly generated channels with different porosities (rightmost plot).

During the outbreak of the COVID-19 epidemic we became actively involved in the ICT research that could help in modelling the intensity of interpersonal contacts. We extended the P2-0016 research program by investigating the user-centric approach to exploit the features of wireless networks with the main aim to estimate the "contact intensity" of a user with other user(s) (or infected person(s)). Using the developed mobile application and associated data platform, for monitoring the "radio environment", in this research, we addressed the "contact intensity" between people/devices and investigated innovative methods for estimating the "contact intensity" based on the footprint of the radio environment recorded by the user device. We focus on technology that can be monitored with mobile phones, especially Wi-Fi and BLE. The preliminary results, evaluating the effectiveness of the proposed approach, were presented at conferences.

The laboratory is also part of a new COST Action CA 20210 INTERACT "Intelligence-enabling radio communications for seamless inclusive interactions" launched in 2021. It aims to achieve scientific breakthroughs by introducing novel design and analysis methods to make future radio-communication networks intelligent, i.e., aware, adaptive, and parsimonious, and to contribute to the creation of intelligent environments. We participate in the three work groups, namely, "Radio Channels", "Signal Processing and Localization", and "Network Architectures and Protocols", horizontal activities including "Data Sets" and "Dissemination and Training", and in the vertical team "Smart Buildings and Cities".

We have continued research in the field of the Internet of Things (IoT). We have extended the LOG-a-TEC experimental testbed with functionalities that support experimentation with BLE technology, with the primary interest in localization and distance between BLE devices. The research was focused on RSSI-based solutions for an estimation of "contact intensity" in an outdoor environment, which is a very challenging task and critical in epidemic conditions, as well as on interference avoidance in 6TiSCH (IPv6 over TSCH mode of IEEE 802.15.4e) wireless technology for the Industrial Internet of Things (IIoT).

In the signal-processing area, we continued to perform comprehensive statistical analyses of signal rain attenuation and fade duration obtained from three years of Alphasat satellite beacon measurements. Complementary

> **ARRS recognised the scientific achievement titled "Personalised Real-Time Control of Hidden Temperature Variables in Therapeutic Knee Cooling" within the project promotion of science – Excellence in Science for 2021.**

> **Blaž Bertalanič received best-student-paper award as the first author of the contribution "A deep learning model for anomalous wireless link detection" presented at the IEEE International Conference on Wireless and Mobile Computing, Networking and Communications (WiMob).**

cumulative distribution functions (CCDFs) of rain attenuation for each year individually and for the three years combined were published in high-impact journals. In addition, signal processing expertise was used to address the problem of identifying the network topology in low-voltage power distribution grids. We investigated the shortcomings of existing methods and presented a new approach to topology identification that avoids the assumption of linearized power flow. We succeeded in reducing the sensitivity of the reconstruction process to the measurement errors and successfully reconstructed the experimental low-voltage grid topology from smart-meter measurements.

In the **Parallel and Distributed Systems Laboratory**, we continued developing local mesh-free methods for the numerical solving of systems of partial differential equations (PDEs). In 2021 we implemented a prototype p-adaptive solution procedure. Based on promising results, we initialised research of a completely automatic p-adaptive approach. We developed an original parallel algorithm for the discretisation of parametric surfaces – an important step towards the coupling of mesh-free analysis and Computer Aided Design (CAD). Furthermore, we developed a dimension independent refined mesh-free solution to non-Newtonian natural convection, where we demonstrated the obvious gain in computational efficiency of the refined solution. In collaboration with the University of Wroclaw, we started research on inertial effects on fluid flow in complex porous media, where we plan to perform systematic numerical studies of the flow through complex porous media to account for hydraulic tortuosity. Finally, we used developed techniques for the implementation of an applied research project (mentioned later) dealing with plastic deformation.

Figure 3: Gramian angular summation field-based representation of wireless-link layer anomalies

We continued our collaboration with the Geological Survey of Slovenia and the University of Ljubljana, Faculty of Arts, Department of Geography on the ARRS project "J1-2479 - Past climate change and glaciation at the Alps-Dinarides junction", which recognises markers of past glaciations as important archives for the study of Quaternary climate change. In 2021 we prepared the Parallel Ice Sheet Model (PISM) simulation environment and the input data for it, such as digital elevation maps and climate factors. We have also developed a new climate forcing model.

We continued research within the ARRS project "J7-2599 - Decay of an invasive ctenophore bloom as a perturbation to the costal marine microbial community", where our laboratory is engaged in numerical and oceanographic modelling. In 2021 we proposed a novel population-based model for microbial growth based on Monod and Luedeking-Piret models that was used to model the laboratory results of our project partners. The resulting conference paper "A model for jellyfish detritus decay through microbial processing" was awarded the best-paper prize at the Mipro 2021 conference.

In 2021 we started collaborating on four core research projects. Project "N2-0171 - Graph Theory and Combinatorial Scientific Computing" will, in cooperation with the Faculty of Computer and Information Science (FRI), InnoRenew (SI) and the Alfréd Rényi Institute of Mathematics (HU), identify problems related to the Combinatorial Scientific Computing in connection with Graph Theory, and design and implement optimization graph algorithms for solving these problems on massively parallel computers.

In cooperation with the Faculty of Electrical Engineering (FE) and the Communication Technology Laboratory, we started the project "J2-3048 - Advanced modelling of radio channels using ray-optical and numerical meshless methods". The objective of the project is the adaptation/development of a numerical meshless model for the electromagnetic propagation problem that can be successfully applied to smaller radio cells, which are considerably affected by the environment geometry and composition.

> **We published a paper on the use of machine learning for wireless-link quality estimation in the highest-ranked journal in telecommunications area with the impact factor higher than 25.**

In cooperation with the Faculty of Sport and the Laboratory for Machine Intelligence at the Faculty of Electrical Engineering, we launched the project "J3-3115 AiCoachU – Artificial intelligence is coaching you" with the objective to demonstrate a successful recognition of fatigue onset, and excessive pelvic and rearfoot mechanics at different running velocities and surface inclines using a dedicated sensor platform and deep learning.

In collaboration with the F1 department and the Communication Technology Laboratory, we started a project "N2-0171 - Cryptographically secure random number generator", where we plan to develop a cryptographically secure generation of pseudo-random numbers. For the purpose of generating randomness, the module will enable capturing entropy from the sources offered by the operating system, from the hardware of the mobile device and from the user's actions.

In 2021 ARRS recognised the scientific achievement titled "Personalised Real-Time Control of Hidden Temperature Variables in Therapeutic Knee Cooling" within the project promotion of science – Excellence in Science for 2021.

In the scope of applied research, we continued the development of DiTeR – a modular dynamic thermal rating (DTR) software designed to predict the thermal state of power lines, which is in operational use at ELES, ltd. and it is marketed world-wide by the company Operato. In the scope of the maintenance contract and additional consultant contract, we improved the Uncertainty module for DTR and performed analyses of microscale weather modelling that is crucial for accurate DTR forecasts.

In 2021 we expanded our participation in the field of power systems by starting two applied research projects. The project "TrafoFlex: advanced concept for the efficient use of transformers leveraging the DTR technology" deals with developing and testing the concepts of advanced use of transformers in terms of operation, flexibility and asset management. Our role in the project is the development of the DTR physical model for power transformers for the company Operato.

For the Diagnostics and Analytics Centre (DAC) at ELES, ltd., we started a project "Forecasting maintenance interventions of the on-load tap changer with advanced analytics", where our job is to develop a prediction model from the number of switching operations based on domain knowledge, statistics, and machine learning, and deploy software implementation of the model into operative use for DAC.

In 2021 we also completed two smaller applied projects for the National Institute of Biology (NIB) and the Austrian company SinusPRO. For NIB, we performed a coupling of the oceanographic model CROCO and the biogeochemical model BFM libraries. For SinusPro GmbH, we dealt with a meshless simulation of the plastic continuum deformation arising during the 3D-printing process. We modelled the plastic deformation using the von Mises plasticity model with non-linear isotropic hardening.

The research in the **Networked Embedded Systems Laboratory** is primarily focused on the integration of sensor, communication, computing and data technologies to support the digitalization of verticals and the operation of smart infrastructures with the aim to improve their accessibility, utility and efficiency of resource utilisation. To this end we are making use of contemporary concepts such as service-oriented architecture, dynamic service composition, cognitive communications, Internet of Things, machine learning and deep learning.

In the frame of the research programme P2-0016 (Communication networks and services) we continued with the investigation and adaptation of machine- and deep-learning methods for advanced data-driven radio resource management, with special attention to transfer learning, self-supervised learning and alternative techniques for representation of time series data. In addition to commonly used techniques for dimensionality reduction to the most representative features for motif recognition and classification we started the investigation of methods for dimensionality extension with the aim to improve anomaly and motif recognition in time series. We also continued the development and investigation of procedures for the lifecycle automation of smart infrastructures with the support of artificial intelligence, focusing on the deployment and operations phases. In particular we were working on the procedures for automated initial provisioning and in-operation service upgrade based on zero-touch and voice-assisted approaches.

In 2021 we also continued with the research work in the H2020 projects SAAM, Fed4FIRE+, RESILOC and BD4OPEM, as well as in the basic research project funded by the Slovenian Research Agency J2-9232 LoLaG.

We successfully concluded research activities in the SAAM (Supporting Active Ageing Through Multimodal Coaching) project, where we further enhanced the algorithms and piloting functionalities for multimodal activity and context monitoring via the energy consumption of home appliances and interference in the UWB radio channel, and supported further pilot deployments of unobtrusive sensing for monitoring and identifying the activity of the elderly population in real home environments.

As part of the Fed4FIRE+ (Federation for FIRE plus) project we extended the LOG-a-TEC experimental testbed with the IEEE 802.15.4 ultra-wideband (UWB) technology supporting short-range, low-power communications and channel impulse response (CIR) measurement and ranging to enable experiments on precise indoor and outdoor localization and tracking, motion and object detection, interference analysis, etc. By introducing the concept of continuous deployment of experiments, which supports simultaneous execution of parallel experiments and their fully automated execution, we also simplified user interaction with the testbed.

In RESILOC (Resilient Europe and Societies by Innovating Local Communities) we continued the work on IoT and wireless-networking-based solutions for improving the resilience indicators of local communities to different disasters and unexpected events. We finalized the design and implementation of (i) a low-cost electronic tag with Bluetooth beaconing for the identification of people and assets; (ii) a mobile app for the anonymised crowdsensing of people's movement and carrying out short surveys / opinion polls before and after the adoption of new resilience measures; (iii) a Bluetooth and Wi-Fi radio sniffing gateway for the indirect monitoring of people's behaviour and movement; and (iv) a back-end system with communication protocols, databases and APIs to efficiently support the integration of developed solutions into the RESILOC cloud platform. We also contributed in the specification of use cases for the above solutions in the frame of planned trials in local communities.

In 2021 we continued the research activities in the BD4OPEM project (Big Data for OPen innovation Energy Marketplace) with participation in the design and implementation of the architecture for an open, modular and scalable data-analytics marketplace and the methodology for the acquisition and treatment of large quantities of data from various sources. The main focus was on the development of services for the flexible aggregation of demand and response and services supporting an insight into and the management of distributed energy production and consumption in smart buildings and industry. The objective of these data-driven services is efficient and automatic management of distributed renewable energy sources and loads for shifting or reduction the peak energy demand and the fluctuations in transport and distribution as well as the optimization of energy consumption to fluctuating power tariffs.

In 2021 we also successfully concluded the basic ARRS project J2-9232 – LoLaG (Resource management for low latency reliable communications in smart grids), in which we tested and validated the suitability of the developed edge-cloud computing framework for automated real-time fault localization in distribution networks using phasor measurement units (PMUs) as edge devices, thus avoiding additional communication delays and potential data losses due to transfer to the cloud.

Some outstanding publications in the past year

1. G. Morano, A. Hrovat, M. Vučnik, J. Puhan, G. Gardašević, D. Vasiljević, T. Javornik. Experiment control and monitoring system for LOG-a-TEC testbed. Sensors. 2021, vol. 21, no. 19, str. 6422-1-6422-16. ISSN 1424-8220, DOI: 10.3390/s21196422.

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3. T. Kocevska, T. Javornik, A. Švigelj, A. Hrovat. Framework for the machine learning based wireless sensing of the electromagnetic properties of indoor materials. Electronics. 2021, vol. 10, no. 22, str. 2843-1-2843-24. ISSN 2079-9292, DOI: 10.3390/electronics10222843.

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6. J. Slak, G. Kosec; Medusa: A C++ library for solving PDEs using strong form 1 mesh-free methods, ACM transactions on mathematical software, vol. 47, 2021, DOI: 10.1145/3450966.

7. A. Rashkovska, R. Trobec; Framework for personalized real-time control of hidden temperature variables in therapeutic knee cooling, IEEE journal of biomedical and health informatics, vol. 25, 2021, DOI: 10.1109/JBHI.2020.3005480.

8. Cerar, Gregor, Yetgin, Halil, Mohorčič, Mihael, Fortuna, Carolina. Machine learning for wireless link quality estimation : a survey. IEEE Communications surveys and tutorials, ISSN 1553-877X, 2021, vol. 23, iss. 2, str. 696-728, ilustr., DOI: 10.1109/COMST.2021.3053615.

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INTERNATIONAL PROJECTS

1. Implementing Plasticity Model in FreeFEM++
Dr. Gregor Kosec
Sinuspro GmbH

2. COST CA18203; ODIN - Optimising Design for Inspection
Dr. Gregor Kosec
Cost Association Aisbl

3. COST CA20120 - INTERACT; Intelligence-Enabling Radio Communication for Seamless Inclusive Interactions
Prof. Tomaž Javornik
Cost Association Aisbl

4. H2020 - Fed4FIREplus; Federation for FIRE Plus
Prof. Mihael Mohorčič
European Commission

5. H2020 - SAAM; Supporting Active Ageing through Multimodal Coaching
Prof. Mihael Mohorčič
European Commission

6. H2020 - RESILOC; Resilient Europe and Societies by Innovating Local Communities
Prof. Mihael Mohorčič
European Commission

7. H2020 - BD4OPEM; Big Data for Open Innovation Energy Marketplace
Prof. Mihael Mohorčič
European Commission

8. Joint Scheduling and Routing Algorithm for Delay Sensitive Industrial Applications in Wireless Networks
Asst. Prof. Andrej Hrovat
Slovenian Research Agency

9. Machine Learning Supported Indoor Localization
Dr. Klemen Bregar
Slovenian Research Agency

RESEARCH PROGRAMMES

1. Communication networks and services
   Prof. Mihael Mohorčič
2. Parallel and Distributed Systems
   Dr. Gregor Kosec

R&D GRANTS AND CONTRACTS

1. Past climate and glaciation at the Alps-Dinarides junction
   Dr. Gregor Kosec
2. Decay of an invasive ctenophore blooms as a perturbation to the coastal marine microbialcommunity - from molecules to ecosystem - an integrated interdisciplinary approach
   Dr. Gregor Kosec
3. Graph Theory and Combinatorial Scientific Computing
   Dr. Matjaž Depolli
4. AiCoachU – Artificial intelligence is coaching you
   Dr. Gregor Kosec
5. Resource management for low latency reliable communications in smart grids – LoLaG
   Prof. Mihael Mohorčič
6. Towards the environment-aware intelligent wireless communications
   Prof. Aleš Švigelj

7. Advanced modelling of radio channels using ray-optical and numerical meshless methods
   Prof. Tomaž Javornik
8. Cryptographically secure random number generator
   Dr. Matjaž Depolli
9. Cryptographically secure random number generator
   Dr. Matjaž Depolli
   Government Office of the Republic of Slovenia for the Protection of Classified Information
10. CROSSING - Crossing Borders and Scales - An Interdisciplinary Approach
    Dr. Matjaž Depolli
    Helmholtz-zentrum Dresden-Rossendorf E.v.

NEW CONTRACTS

1. DTR software: DiTeR
   Dr. Gregor Kosec
   Eles, d. o. o.
2. Forecasting maintenance interventions of the on-load tap changer with advanced analytics
   Dr. Gregor Kosec
   Eles, d. o. o.

VISITOR FROM ABROAD

1. Ljupcho Milosheski, Prilep, North Macedonia, 19. 4. –17. 7. 2021

STAFF

Researchers
1. *Dr. Viktor Avbelj, retired 01.08.21*
2. Dr. Andrej Čampa*
3. Dr. Matjaž Depolli
4. Dr. Carolina Fortuna
5. Dr. Ke Guan
6. Asst. Prof. Andrej Hrovat
7. Prof. Tomaž Javornik
8. *Prof. Monika Kapus Kolar, retired 02.11.21*
9. Dr. Gregor Kosec
10. Prof. Andrej Lipej*
11. **Prof. Mihael Mohorčič, Head**
12. Asst. Prof. Roman Novak
13. *Dr. Igor Ozimek, retired 02.08.21*
14. Dr. Aleksandra Rashkovska Koceva
15. Prof. Aleš Švigelj
16. *Dr. Halil Yetgin, left 22.03.21*
Postdoctoral associates
17. Dr. Klemen Bregar
18. Dr. Gregor Cerar
19. Dr. Arsim Kelmendi*
20. Dr. Sebastijan Mrak
21. *Dr. Jure Slak, left 07.06.21*

22. *Dr. Matevž Vučnik, left 01.11.21*
Postgraduates
23. Blaž Bertalanič, B. Sc.
24. Marko Hudomalj, B. Sc.
25. Mitja Jančič, B. Sc.
26. Grega Morano, B. Sc.
27. Miha Rot, B. Sc.
28. Denis Sodin, B. Sc.
29. Filip Strniša, B. Sc.
Technical officers
30. Viktor Cvrtila, B. Sc.
31. Miha Mohorčič, B. Sc.
32. Din Mušić, B. Sc.
33. Miha Smolnikar, B. Sc.
Technical and administrative staff
34. Polona Anžur, B. Sc.
35. Tomaž Krištofelc
36. Tamara Matevc, B. Sc.
37. Marko Mihelin*, B. Sc.

Note:
* part-time JSI member

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ORIGINAL ARTICLE

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12. Roman Novak, "Three-point synchrophasor estimator with better off-nominal frequency leakage reduction", *IEEE access*, 2021, **9**, 50126-50137.

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22. Andrej Lipej, "Flow conditions influence on the instability of a pump characteristic", *Journal of applied fluid mechanics*, 2021, **14**, 4, 1249-1255.

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22. Blaž Rojc, Matjaž Depolli, "A resizable C++ container using virtual memory", In: *ICSOFT 2021, 16th International Conference on Software Technologies, July 6-8, 2021*, Proceedings, Science and Technology Publications, 2021, 481-488.

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THESES AND MENTORING

1. Gregor Cerar, *Classification of wireless links using machine learning techniques:* doctoral dissertation, Ljubljana, 2021 (mentor Mihael Mohorčič; co-mentor Carolina Fortuna).

COMPUTER SYSTEMS DEPARTMENT
E-7

The Computer Systems Department is concerned primarily with the development of efficient optimization algorithms, intelligent massive-data processing, effective data management and visualization, and adaptive computing structures for the faster and more reliable execution of algorithms. Within this broad area, we are concentrating on self-adapting systems, the modelling and optimizing of complex, dynamic and non-deterministic systems. Our research results are implemented within applications for production, transport, bioin formatics, nutrition, 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 remain at the forefront of rapidly developing fields.

Head:
Prof. Gregor Papa

In 2021 we continued with the work on our research programme (Computer Structures and Systems – P2-0098), funded by the Slovenian Research Agency. The programme is focused on relevant research and development in the areas related to reconfigurable systems: reliability, architectures for data-intensive systems, hardware/software co-design, resource planning and scheduling, adaptive and learning control methodologies, dynamic adaptation to changing contexts, decision and control in uncertain and changing environments. The interdisciplinary state-of-the-art research challenges combine fields from computer science, engineering and mathematics. Our research work in 2021 was complemented by the design, development and implementation of various solutions within 12 European projects in *Horizon 2020, ECSEL JU, EFSA* and *Interreg* programs, as well as in 4 national projects. Our work is also actively connected to the activities of the Slovenian *Strategic research and innovation partnerships (SRIP)* in the domains of *Smart cities and communities (SC&C)* and *Factories of the future (FoF)*.

Optimization algorithm design

Many real-world application areas involve the optimization of several, often time-consuming and conflicting objectives. They may require the use of computational intelligence, for example, for the maximization of the quality while minimizing the cost, relying on demanding numerical simulations.

Worst-case scenario optimization deals with the minimization of the maximum output in all scenarios of a problem, and it is usually formulated as a min-max problem. Employing nested evolutionary algorithms to solve a problem requires numerous function evaluations. We proposed the use of a differential evolution with an estimation of distribution algorithm. To reduce the computational cost we estimate the distribution of the best worst solution for the best solutions found so far. The probabilistic model is used to sample part of the initial population of the scenario space differential evolution, using a priori knowledge of the previous generations. The work was published in the *Mathematics* journal. The multi-population pessimistic bilevel optimization approach was presented at the *International Conference on Evolutionary and Deterministic Methods for Design, Optimization and Control – EUROGEN 2021*.

We are developing an indoor localization solution using smartphones without the use of a network and satellite navigation

Part of the research was focused on applying **gradient-based methods** to machine learning and large-scale optimization. The exploration of the effectiveness of gradient-based methods was performed in different branches of machine learning: supervised, unsupervised and reinforcement learning. In the scope of this work a lecture on deep learning with Keras was given at the *Summer School on Data Science – SSDS 2021*. Furthermore, as a non-negative matrix tri-factorization (NMTF) problem has a special importance in data science, since it serves as a mathematical model for the fusion of different data sources in data clustering, we developed different methods, one also based on the adaptive moment estimation method. Numerical results show that with sufficient computing time the method performs satisfactorily. The work was published in the *Journal of Global Optimization*.

In the ARRS young-researcher project, the focus was on algorithms, benchmarking, **exploratory landscape analysis**, data visualization and machine learning. This resulted in two conference papers on data management and visualization presented at the *IEEE Congress of Evolutionary Computation – CEC 2021*, and the *Genetics and Evolutionary Computation Conference – GECCO 2021*. Also, a journal paper on data processing and machine learning was published in the *Mathematics* journal.

We have proposed a new pipeline for the landscape analysis of **time-series machine learning** datasets that enables us to better understand a benchmarking problem landscape, allows us to select a diverse benchmark datasets portfolio, and reduces the presence of a performance assessment bias via bootstrapping evaluation. Combining a large multi-domain representation corpus of time-series specific features and the results of a large empirical study of time-series classification (TSC) benchmark, we showcase the capability of the pipeline to point out issues with non-redundancy and representativeness in the benchmark. By observing discrepancy between the empirical results of the bootstrap evaluation and recently adopted practices from the TSC literature when introducing novel methods, we warn of the potentially harmful effects of tuning the methods on certain parts of the landscape (unless this is an explicit and desired goal of the study). Finally, we propose a set of datasets uniformly distributed across the landscape space one should consider when benchmarking novel TSC methods. The research was published in the *Expert Systems with Applications* journal.

Figure 1: Benchmark problems (*red*) cover only a very small space when compared to the artificially generated problems (*black*)

As a part of the ARRS post-doc project *Mr-BEC – Modern approaches for Benchmarking in Evolutionary Computation* (http://cs.ijs.si/project/mrbec), we have followed the idea of **robust statistical methods** that can be used for single-objective optimization to develop the multi-objective Deep Statistical Comparison (DSC) approach. We have proposed a novel ranking scheme that reduces the bias in the user-preference selection by comparing the high-dimensional data of approximation sets, and consequently provides more robust statistical results. This approach was presented at the *GECCO 2021*. In addition, the DSC approaches have been used to develop, in collaboration with the Leiden University, the Netherlands, a new ensemble for comparing multi-objective optimization algorithms using multiple performance measures, presented at the *International Conference Series on Evolutionary Multi-Criterion Optimization – EMO 2021*. To show the transferability of the approach to other research domains, we have transferred the use of the DSC approaches to benchmarking recommender systems, published in the *Big Data Research* journal, and in natural-language processing scenarios in order to provide general recommendations for deep learning architectures suitable for a new application scenario, published in the *IEEE Access* journal.

We have explored the characteristics that can be used for describing single-objective optimization problems with regard to their robustness of problem transformations (e.g., shifting, scaling), presented at *CEC 2021*. To find the relations between the problem characteristics and the performance achieved by the algorithms, we have developed several machine-learning pipelines that can be used for the automated algorithm prediction and selection, and were presented at the *GECCO 2021*, *IEEE Series Symposium on Computational Intelligence – SSCI 2021* and *Applications of Evolutionary Computation – EvoApplications 2021.* At the latter event, our contribution won the Best Paper Award.

To support reproducible results of the studies and easy sharing of the data involved in ML experiments, we have developed *OPTION*, which is optimization algorithm benchmarking ontology, and was presented at the *GECCO 2021*. This ontology provides the vocabulary needed for the semantic annotation of the core entities involved in a benchmarking process, such as algorithms, problems and evaluation measures.

In cooperation with the Department of Intelligent Systems at the JSI and the Faculty of Electrical Engineering and Computer Science, University of Maribor, we organized, for the eighteenth consecutive year, the *Nature-inspired algorithms* workshop, dealing with stochastic optimization techniques.

We organized workshops and a special session on benchmarking at the *GECCO 2021* and *CEC 2021*, and on representation learning at *CEC 2021*. An invited talk on automated algorithm performance prediction was given at *ETAI 2021*. At the *GECCO 2021* and *CEC 2021* we provided a tutorial about statistical analyses of single-objective optimization algorithms. As a contribution to a more systematic use of **dynamic control parameter** choices for evolutionary computations, we gave a tutorial during the *GECCO 2021* conference. We surveyed the existing techniques to automatically select control-parameter values on the fly. In addition, we discussed both theoretical and experimental results that demonstrate the unexploited potential of dynamic parameter choices.

We acted as editors and guest editors at regular and special issues of various journals, i.e., *Natural Computing*, *Sensors*, *Automatika*.

Data processing

Electronic components and systems (ECSs) are essential to the economy and citizens of the EU, supporting several fields ranging from transport and mobility to medicine and energy. One key area to be addressed is **enhancing the reliability** of ever more complex chips and systems designed to handle huge amounts of data

while delivering greater processing speed and accuracy and decreasing energy consumption. Reliability will be increasingly important in the era of Industry 4.0 and the Internet of Things with cloud-connected real-time data processing underlying 'mission-critical' applications such as self-driving cars. In 2020 we started with the ECSEL JU / Horizon 2020 project *iRel40 – Intelligent Reliability 4.0* (https://www.irel40.eu) in collaboration with 75 partners from 13 countries to reduce the failure rates of ECSs all along the value chain. Our department contributes to the realization of the smart condition monitoring system for in-wheel electric motors developed by Elaphe, a Slovenian automotive company that is moving the boundaries with their development of compact, high-torque electric motors that fit inside a wheel and can operate in the toughest of conditions. The research in iRel40 will enable motor lifetime prediction, using smart sensing and on-line data monitoring technologies, as well as detection of possible degradation of critical components. We are applying state-of-the-art AI methods to achieve this, especially by using deep neural networks to identify critical parameters that have the greatest impact on the

Mobile application Eatvisor provides insights into the nutritional values of specific foods

motor health, and to detect possible motor failure before it happens. Our focus is on the prediction of the winding insulation resistance of a motor, which was proven to be the most critical indicator implying failure, using standard on-line measurements of the motor that can be carried out even during the motor operation. Reliability is especially important in such innovative applications where a fundamental understanding of the physics of failure is still lacking in the literature, specifically when the system faces exceptional environments such as extreme temperatures. To this end, we are employing machine learning methods to model the motor behavior with respect to environmental parameters as well as electrical ones to push the overall quality levels and reliability specifically. We are making use of the most advanced techniques in artificial intelligence to capture the physical characteristics of motors even in the far-from-ideal conditions such as large measuring noise, concept drift due to accelerated aging, unknown modes of failure, temporal correlation and others.

Being both a poison and a cure for many lifestyle and non-communicable diseases, food is becoming the prime focus of precision medicine. The monitoring of a few groups of nutrients is crucial for some patients, and methods for easing their calculations are emerging. Our proposed machine-learning pipeline deals with **nutrient prediction based on learned vector representations** of short text-recipe names. We explored how the prediction results change when, instead of using the vector representations of recipe descriptions, we use the embeddings of the list of ingredients. The nutrient content of a food depends on its ingredients; therefore, the text about the ingredients contains more relevant information. We define a domain-specific heuristic for merging the embeddings of the ingredients, combining the quantities of each ingredient in order to use them as features in machine learning models for nutrient prediction. The results from the experiments indicate that the prediction results improve when using the domain-specific heuristic. The prediction models for protein prediction were very effective, with accuracies of up to 97.98 %. Implementing a domain-specific heuristic for combining multi-word embeddings yields better results than using conventional merging heuristics, with its accuracy higher by up to 60 % in some cases. Our work on this topic was published in the *Mathematics* journal.

We introduced a new semantic similarity heuristic, based on **sentence vector embeddings**. Additionally, we extended the evaluation by taking real-world examples and tasking a subject-matter expert to rate the relevance of the top three matches for each example. The results show that using semantic similarity with the sentence embedding method yields the best results, achieving an 88 % accuracy for a ground truth data set and a 91 % accuracy of the human-expert evaluation, while the lexical similarity heuristic provides comparable results with 75 % and 85 % accuracy. The work was presented at the *International Joint Conference – BIOSTEC* 2021.

We continued with our activities in ECSEL JU / Horizon 2020 project *InSecTT – Intelligent Secure Trustable Things* (https://www.insectt.eu/) with 52 partners involved, bringing together the Artificial Intelligence (AI) techniques and the Internet of Things (IoT). It is devoted to fostering the cooperation between big industrial players from various domains, a number of highly innovative SMEs distributed all over Europe and cutting-edge research organizations and universities. Our department participates in two use cases. The first use case is related to smart and adaptive connected solutions across the health continuum within a smart hospital where we are working on developing anomaly-detection methods relating to patient biomedical signals, using deep neural networks (DNNs). We used a large anonymized public database containing over 40.000 annotated ECG signals to train and test several DNN models for anomaly detection. We concentrated on the supervised learning methods as well as unsupervised methods, like generative adversarial networks (GANs). Reliable anomaly detection will help us to assess a patient risk profile needed to allocate the necessary hospital resources to a particular patient. It will be integrated into the use-case architecture together with the solutions from other use-case partners.

The second use case is related to emergency logistic services in healthcare where we are developing an indoor localization solution, using a smartphone without a network and satellite navigation. We developed an android app to support rescue teams in emergency situations such as mass-casualty incidents. Using only prepositioned

QR codes, the app is able to determine the indoor location of a user and then send this information together with the triage decision made by the first responders to the cloud, where it remains available to the other rescue team members, thus facilitating picking up casualties. The app is also capable of a basic indoor navigation at a floor level getting all the necessary information, like the floor plan, possible destinations and navigation graphs from the QR code positioned at the floor entrance. In both use cases we focus on developing and using explainable and trustworthy AI methods which help users to understand the reasons for the outcomes of specific procedures.

More than 30 billion sensor-equipped IoT devices provide a flurry of multimodal data. Together with advanced machine learning-based processing, these data may uncover various aspects of human behavior. Understanding the user's cognitive load, for instance, is critical for improved human-computer interaction (HCI), yet, inferring the cognitive load from opportunistically sensed data remains challenging, with only a handful of experimental approaches developed and none being independently evaluated. Our work on consolidating the area of cognitive load inference via mobile sensing was published in the *IEEE Access* journal. We collected a rich dataset of multimodal data acquired via wearable sensing as the users were solving tasks of varying difficulty, and annotated the dataset with the user's (subjective and objective) cognitive load effort. We then organized an international machine-learning challenge where 13 entries competed in inferring cognitive load on a held-out part of our dataset. Our efforts have not only drawn together top researchers in HCI, ML, and ubiquitous computing, but also derived actionable guidelines for future cognitive load inference systems. In parallel, we also tacked the problem with wireless sensing and developed a

Figure 3: Automated guided vehicle (produced by TPV Company) was upgraded with an additional camera to allow for more intelligent behavior and object avoidance

software-defined radio-based system for cognitive load inference, as published in *International journal of human-computer interaction*. The work shows that wireless cognitive load inference can provide the performance that is on par with that provided by more intrusive wearable devices.

Data management and visualization

We continued with the upgrade and improvement of the **national food composition database** using the database and knowledge-base management system that are the key parts of the *Open platform for clinical nutrition – OPEN* (http://www.opkp.si). Our aim is to provide food and nutrition experts with an easy way to browse, maintain and integrate food and nutrition data. We designed and implemented a user interface, which allows users to connect nutrient values with the information about food items, food groups and tags borrowed from multiple food databases (USA, IT, NL, etc.). The developed data and knowledge-base management system form an easy-to-use tool, where experts can easily search through different food and nutrition databases, edit them and further link the nutrition information to the chain of data. The designed tool also allows the user to quickly and intuitively review and correct nutrition data, which can be very helpful when reviewing large amounts of such data. In this way we did not only increase the predictability of the tool and help nutrition specialists to find data as quickly as possible, but we also ensured that all the future data in our database would have a unified way of visualization.

The obtained data from the OPEN database will be further used for the iOS and Android mobile application *Eatvisor* that we are currently developing. It provides insights into the nutritional values of specific foods; it allows barcode scanning of branded products, writing your own recipes, comparing different foods, logging physical activities and writing food diaries (also using deep learning approaches). In addition, it can be used by the experts for diet and meal planning for healthy individuals, athletes, diabetics and patients. *Eatvisor* was co-designed with a team of nutrition experts, computer scientists, graphical designers and end users.

We completed the development of the web-based tool *Šolski lonec* (http://solskilonec.si), which is currently being tested at 20 different primary schools. Our goal is to enable nutrition experts to plan balanced meals that are consistent with national nutrition guidelines and recommendations. We designed interactive visualizations that help experts determine the appropriate amounts of individual food groups and specific nutrients, which can be achieved by searching and inputting multiple food items from the *OPEN* database, or by manually inputting the required data about the food items not already included in the *OPEN* database. Moreover, the tool enables users to compose and modify their own recipes and calculate how much food and how many meals they need to prepare based on the pre-entered data of final users (e.g., students, pupils, etc.). Nutrition experts can very clearly and quickly check whether designed menus follow the national dietary guidelines.

We started with another Horizon 2020 project, *COMFOCUS – Community on Food Consumer Science* (https://comfocus.eu), with the vision that Open Science is the basis for food consumer science, which will become

future-proof. Our role in the project is to support food consumer scientists in the normalization and **fusion of heterogeneous data** collected by various studies measuring and testing consumer behavior and preferences. For the analysis of the fused data, analytical techniques from machine learning (e.g., ensembles of methods, meta-learning, supervised and unsupervised learning), deep learning and statistics will be applied. In collaboration with food consumer scientists, we defined ontology modeling concepts and entities defining consumer behavior and preferences.

We continued with the Horizon 2020 project called *FNS-Cloud – Food Nutrition Security Cloud* (http://www.fns-cloud.eu) where we consolidated the existing FNS resources (data, knowledge and tools) for health and agri-food sciences, which were fragmented, lacking critical mass, and their access by user communities was 'unevenly' distributed. Particularly, we developed an advanced methodology to work with heterogeneous data on food, nutrition and health. Our group has been working on the methodologies for data **standardization and interoperability of data** on food and nutrition security, including specific tasks on data pre-processing, data curation and annotation, data matching and data analysis.

As a part of the FNS-Cloud H2020 project and an EFSA-funded project called *CAFETERIA – ExtraCting and Annotating Food NamEd EnTitiEs fRom ScIentific LiterAture*, we explored corpus-based named-entity recognition methods that can be used for extracting food entities from textual data (i.e., recipes or scientific abstracts). For this purpose, we fine-tuned the recent advances in natural language processing (NLP) to develop NER methods that can extract food entities and, at the same time, also perform named-entity linking by assigning semantic tags from different food ontologies and resources; this work was published in the *Journal of Medical Internet Research*. In addition

> **We developed an advanced methodology to work with heterogeneous data on food, nutrition and health**

we developed the first relation extraction method that can be used for extracting the relation between food and biomedical entities from textual data. This method uses transfer learning in order to support recent advances in the NLP for relation extraction, and was presented at *Workshop on Biomedical Language Processing – NAACL 2021*. Its utility was shown when extracting food-disease and food-chemical relations, and was presented at the *SSCI 2021*.

As a part of the FNS-Cloud H2020 project we developed, in collaboration with the Department of Knowledge Technologies, a text mining pipeline, *DietHub*, which can be used to automatically assign ingredients to a recipe description, and it was published in the *Trends in Food Science & Technology* journal. This was further used to analyze recipes consumed before and during the first Covid-19 isolation, which helped us to identify changes in the food consumption patterns (this research won the award *Odlični v znanosti* (Excellence in Science) presented by the ARRS for 2021). In addition, we have been involved in a study that analyzes the Covid-19 impact on eating behaviors across 16 European countries, which was published in the *Food Quality and Preference* journal.

We organized the Big Food and Nutrition Data Management and Analysis – BFNDMA 2021 at the *IEEE BigData 2021* conference, and the AI & Food and Nutrition track at the *Applied Machine Learning Days – AMLD 2021* event, and an invited talk on food information extraction and data normalization was given at the *IberHeLT 2021* workshop at *SEPLN2021*.

We contributed to the ESFRI project *MetroFood – Infrastructure for Promoting Metrology in Food and Nutrition* (https://www.metrofood.eu). In collaboration with the Department of Environmental Sciences, we helped develop the MetroFood platform and perform data management. Within the Slovenian node, we started designing the Slovenian MetroFood national node.

In the area of **efficient interaction systems**, we focused on the web tools and mobile apps for nutrition and food informatics. We investigated and designed visual representations for various projects, applications and web pages. In collaboration with partners and end-users, we analyzed user needs, defined appropriate user experiences and designed corresponding interfaces for several tools related to nutrition.

We finished our work in two Horizon 2020 projects: *TRUE – Transition paths to sustainable legume based systems in Europe* and *TomRes – A novel and integrated approach to increase multiple and combined stress tolerance in plants using tomato as a model*. Both projects form the agricultural domain share the need for a decision support system. In collaboration with the Knowledge Technologies Department, we designed and implemented a web-based decision support system that enables multiple actors to work collaboratively on the same decision problem, make an assessment of the current state and perform bottom-up and top-down analysis testing different scenarios and finding the way to reach the desired outcome. The research work resulted in the release of two web applications: **Pathfinder** (http://pathfinder.ijs.si/) that aids an assessment and analysis of legume value chains (project True) and **Resource Amplifier** (http://resourceamplifier.ijs.si/) for tomato production (project TomRes). The tools were designed and implemented to be reused in new projects that need decision support based on the qualitative data from experts (not only in the field of agriculture). The generic tool is called **DEXiWare**, as it is based on the existing DEXi methodology and enables its online use. A landing page for dissemination and exploitation was built: http://dexiware.ijs.si/

We continued with the development of the **VešKajJeš** application and its complementary application **VešKajPiješ**. Our department is responsible for the technical aspects related to the mobile application. The application allows users to easily compare food items through the traffic light system and is available on Android and iOS devices. In 2021, the application had about 30,000 active users in Slovenia. The users contributed also more than 10,000 food items to the branded food database, which now includes 40,000 items and is available for commercial use to third parties. Within two major updates in 2021, the functionality of the app was extended with the information about alcoholic beverages and additives such as caffeine and artificial sweeteners. The system to crowd-source data was published in the *Frontiers in Nutrition* journal. The update related to alcoholic beverages was presented at the *11th EUSPR Conference and Members Meeting* and in the *European Journal of Public Health*.

Within the Interreg Program, we started the project SI4Care – *Social Innovation for integrated health CARE of ageing population in ADRION Regions* (https://si4care.adrioninterreg.eu), with the main objective to contribute to the creation of a transnational ecosystem for the social innovation in integrated healthcare services for the ageing population, through a joint collaboration network and a unique strategy translated into regional and national action plans, implemented and monitored within pilots. In collaboration with the Department of Intelligent Systems and the SRIP Smart Cities and Communities, we contributed regional (Slovenia) and sector-specific (research, ICT) input to the challenges addressed by the project. We put our technical expertise at the disposal of project partners who would like to pilot our solutions in their context and started preparations for our own pilots. The biomechanical pilot kicked off at the end of 2021 with the first batch of six participants. We contributed, to the project, the definition and start of a biomechanical pilot with the elderly

Figure 2: Flowchart of the nutrient-value prediction approach

(ongoing) as well as providing information on the status quo and challenges regarding long-term care in Slovenia; a part of this work was presented at the *Alma mater conference* and *Tetramax workshop*.

We concluded the work within the ARRS project *Toponomastic Heritage of Primorska Region* in collaboration with the research group from the Milko Kos Historical Institute of the Research Centre of the Slovenian Academy of Sciences and Arts. Throughout the collaboration we provided computer expertise and support that enabled further improvement of the toponomastic heritage of the Kranjska Region and creation of the toponomastic heritage of the Primorska Region. The final result is a reliable **interactive** version (https://topografija.zrc-sazu.si/) of the Slovenian Historical Topography that includes both regions.

In collaboration with the *Faculty of Sport, University of Ljubljana*, we developed a web application for storage, **management and visualization of scientific literature** and researchers from the area of table tennis. Our role was to create and organize a relational database, and to develop a user interface (UI). The interface allows for user registration and offers different views to users, editors and administrators. Each data class (journal papers, conference papers, books, theses, etc.) has its own view mode enabling quick data searching and filtering. The UI offers several data export possibilities including citation in the APA format, thus representing a useful tool for researchers preparing new publications or gathering information about their research topics.

Adaptive computing platforms

To support and accelerate our algorithms, several approaches were studied and developed at the level of hardware and computing structures, including the use and online reconfiguration of FPGAs, customized embedded systems and sensors. We are building high-performance **FPGA acceleration infrastructure** based on Xilinx ALVEO acceleration cards. We studied the hardware implementations of artificial neural networks on FPGA devices. The use of high-performance ALVEO FPGA acceleration cards was investigated for the fixed-point array multiplication, which can be used in ANNs. The research was also oriented towards quantized neural networks with a focus on algorithms and hardware for their efficient processing. The research, which describes a binarized neural network implemented as a fully combinational circuit on an FPGA, was presented at the *IEEE World Forum on Internet of Things – WF-IoT 2021*. The research is also oriented towards the adaptable delivered quality of computations, i.e., the **approximate computing** approach.

Edge intelligence is currently facing several important challenges hindering its performance, with the major drawback being meeting the high resource requirements of deep learning by the resource-constrained edge computing devices. The most recent adaptive neural network compression techniques demonstrated, in theory, the potential to facilitate the flexible deployment of deep-learning models in real-world applications. However, their actual suitability and performance in ubiquitous or edge-computing applications has not, to this date, been evaluated. In our work, published in the *Electronics* journal, we bridge the gap between the theoretical resource savings promised by such approaches and the requirements of a real-world mobile application by introducing algorithms that dynamically guide the compression rate of a neural network in accordance with the continuously changing context, in which the mobile computation is taking place. Through an in-depth trace-based investigation, we
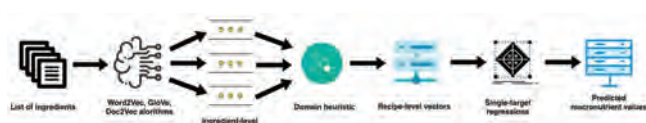
confirm the feasibility of the adaptation algorithms we developed when providing a scalable trade-off between the inference accuracy and resource use. We then implement our approach in real-world edge devices and, through a human activity recognition application, confirm that it provides efficient neural network compression adaptation in highly dynamic environments. The results of our experiment with 21 participants show that, compared to using static network compression, our approach uses 2.18× less energy with only a 1.5 % drop in the average accuracy of the classification.

In the cooperation with *Indian Institute of Technology Indore,* we developed an efficient reusable architecture for the hardware implementation of deep neural networks. In this scope, a sequential Multiply and ACumulate (MAC) unit with arbitrary fixed precision and a reusable Activation Function (AF) unit using multiplexed data paths were developed. The proposed solution reduces the amount of required hardware resource with a negligible additional delay and is suitable for IoT implementations. The solution was tested on a FPGA device as well as simulated for the ASIC implementation. Currently, we are working on the hardware implementation of the Softmax (SF) unit, which is often used in the output layer of a neural network. The work was published in the *Neurocomputing* journal.

In 2021 we started with the ECSEL JU / Horizon 2020 project *DAIS – Distributed Artificial Intelligent Systems* (https://dais-project.eu/) in collaboration with 47 partners from 11 countries. Together we will research and deliver distributed artificial intelligent systems. We tend to solve the problems of running the existing algorithms on these vastly distributed edge devices. Our department aims to develop, in collaboration with Cosylab and TPV, a semi-autonomous automated guided vehicle (AGV) used for transporting materials and products between a factory and its warehouse. We developed the software/hardware needed to retrofit an existing AGV for the data collection process. We already started the data-collection process. We will use this data to train a quantized neural network for object detection, which will help us in our task of developing a semi-autonomous AGV.

In the bilateral project with HZDR, Germany, *CROSSING – Crossing borders and scales: CFD and High-performance computing* (https://www.hzdr.de/db/Cms?pOid=60402&pNid=0), we collaborate on improving the performance of computational fluid dynamics simulations, more specifically population balance equations commonly used in various industrial applications. In real-world systems, there is a need to accurately simulate liquids/solids and interactions between them. One subject of special interest is modelling the size of the bubbles inside a liquid and how they develop during the simulation. Simulations can be arbitrarily complex depending on the used mechanism. The main task was to investigate the possibilities to increase the performance of the so-called class method where bubbles are represented as a discrete distribution. Two of the most important mechanisms changing the bubble-size distribution are coalescence (bubbles merging into bigger ones) and breakup (bubbles breaking up into smaller bubbles). These two mechanisms are extremely computationally expensive and thus require a substantial amount of resources. Graphical processor units (GPUs) were used to substantially increase the performance of the class method by shifting the most expensive and time-consuming calculations from the central processing units to the GPUs. GPU-supported mechanisms can therefore be computed up to two orders of magnitude faster, allowing for a faster model development and reducing the need for expensive/energy-inefficient hardware. This GPU-accelerated approach for calculating coalescence and breakup frequencies was presented at the *International Conference Nuclear Energy for New Europe – NENE2021.*

Within the Horizon 2020 project *SAAM – Supporting Active Ageing through Multimodal Coaching* (http://bilsp.org/saam-active-ageing), the major contributions were the development of **a methodology for estimating the food and nutrient intake** of seniors and the development of an **ambient sensor** with an audio rendering feature. The methodology for food and nutrient intake is based on a short food frequency questionnaire, which was implemented in a mobile (Android) app. An open-source pocket-size kitchen scale that supports the latest Bluetooth technology was developed. It is used to improve the estimation of the food and nutrient intake performed by the mobile app. Additionally, a mobile app for taking and recognizing food and drink from photos was tested. The ambient sensor is a headless system based on an inexpensive Raspberry Pi computer which collects environmental data, like temperature, humidity, pressure and acceleration from the sensor board. Additionally, it collects motion data from wearable sensors via a Bluetooth interface. The acquired data are transmitted to the cloud database system using the MQTT protocol. Besides data acquisition, the ambient sensor integrates an audio rendering feature, voice command module and Moodbox module, which detects the participants' mood by inspecting their voice. Audio rendering is remotely triggered by the coaching system using the MQTT protocol and it plays pre-recorded messages. The developed software (and hardware) is available at the GitHub repository https://github.com/biasizzo/Saam-Rpi-Libra.Scale.

We started to re-brand our open-source kitchen scale Libra (http://libra.ijs.si). By redesigning its visual identity, connecting with possible partners and providing them the supporting visual material (like company stickers that fit on the scale), we started to offer the kitchen scale to a new set of future users. By focusing on analyzing its use, researching the existing field, working out a new frame and executing it, we are designing a website that communicates with potential future users and possible collaborators on the project. We also support them with new visual

materials including photos, icons and other parts of the developed new project identity. The open-source solution of the kitchen scale was presented in the *IEEE Access* journal.

We started a research within the ARRS project *CODA – Context-aware on-device approximate computing* (https://www.fri.uni-lj.si/en/projects/1719) in collaboration with the *Faculty of Computer and Information Science, University of Ljubljana*. The foreseen use case is related to the avalanche-danger mitigation. We started with user requirement specifications and potential stakeholders including backcountry skiers (1000+ responses to an online survey), the Alpine Association of Slovenia and the Environmental Agency of Slovenia (individual interviews).

In the frame of the Horizon 2020 project *TETRAMAX – Technology Transfer via Multinational Application Experiments* (https://www.tetramax.eu) supporting the *Smart Anything Everywhere* European initiative in the domain of **customized low-energy computing** (CLEC) for cyber-physical systems and internet of things, we continued with the activities of the regional Competence Center (CC) within the European-wide network. In cooperation with SRIP SC&C and SRIP FoF, we successfully conducted nine workshops aimed at education and building of the Slovenian ecosystem. Seven of these were the training courses on various topics in the field of CLEC and two events were presentations aimed at the dissemination and building of a local network, at which we presented global trends and our current activities and achievements concerning specific e-Health solutions for the elderly and for a trustworthy use of AI in predictive healthcare.

The Jožef Stefan Institute is a project partner in the Horizon 2020 *Athena* project (https://www.athenaequality.eu/), aiming at removing barriers to the recruitment, retention and career progression of female researchers, lowering gender imbalances in decision-making processes and generating the cultural change needed to avoid gender bias and discriminatory practices through the implementation of Gender Equality Plans (GEPs). To ensure a systemic institutional change, the project plans to conduct an assessment of the procedures and practices already in place in partner organizations, together with an analysis of the national legislation and policy frameworks. In parallel, it will put in place a participatory process aimed, on the one hand, to understand the needs and preferences of the stakeholders and, on the other hand, to train them about selected topics related to gender. As a final result, each partner organization will draft and implement its specific GEP. The *Athena* activities are carried out by nine research departments and Director's Office. The Computer Systems Department participated in collecting data about the current situation in the organization and conducting storytelling interviews. We also participated in the field of promotion; in this role, we launched and promoted an open competition for the Athena logo in the Slovenian region. A representative from our department participates as a member of the GPI Committee, the leading body of the organization, preparing and implementing the GEP. In this role, the representative attended certain compulsory education courses given by the coordinator.

Some outstanding publications in the past year

1. Tome Eftimov, Bibek Paudel, Gorjan Popovski, Dragi Kocev, A framework for evaluating personalized ranking systems by fusing different evaluation measures, *Big data research*, ISSN 2214-5796, 2021, vol. 25, pp. 100211-1-100211-13, doi: 10.1016/j.bdr.2021.100211.

2. Veljko Pejović, Tilen Matkovič, Mojca Ciglarič, Wireless ranging for contactless cognitive load inference in ubiquitous computing, *International journal of human-computer interaction*, ISSN 1044-7318, 2021, vol. 37, pp. 1849-1873, doi: 10.1080/10447318.2021.1913860.

3. Rok Hribar, Timotej Hrga, Gregor Papa, Gašper Petelin, Janez Povh, Nataša Pržulj, Vida Vukašinović, Four algorithms to solve symmetric multi-type non-negative matrix tri-factorization problem, *Journal of global optimization*, ISSN 0925-5001, 2021, vol 82, pp. 283–312. doi: 10.1007/s10898-021-01074-3.

4. Lada Timotijević, Tome Eftimov, Barbara Koroušić Seljak, et al., Designing a research infrastructure (RI) on food behaviour and health: balancing user needs, business model, governance mechanisms and technology, *Trends in food science & technology*, ISSN 0924-2244, 2021, vol. 116, pp. 405-414, doi: 10.1016/j.tifs.2021.07.022.

5. Esther Molina-Montes, Barbara Koroušić Seljak, Robert Modic, Tome Eftimov, Irena Hren, Eva Valenčič, et al., Impact of COVID-19 confinement on eating behaviours across 16 European countries: the COVIDiet cross-national study, *Food quality and preference*, ISSN 0950-3293, 2021, vol. 93, pp. 104231-1-104231-13, doi: 10.1016/j.foodqual.2021.104231.

6. Riste Stojanov, Gorjan Popovski, Gjorgjina Cenikj, Barbara Koroušić Seljak, Tome Eftimov, A fine-tuned bidirectional encoder representations from transformers model for food named-entity recognition: algorithm development and validation, *Journal of medical internet research*, ISSN 1439-4456, 2021, vol. 23, pp. 1-13, doi: 10.2196/28229.

7. Gordana Ispirova, Tome Eftimov, Barbara Koroušić Seljak, Domain heuristic fusion of multi-word embeddings for nutrient value prediction, *Mathematics*, ISSN 2227-7390, 2021, vol. 9, pp. 1941-1-1941-15, doi: 10.3390/math9161941.

8. Margarita Antoniou, Gregor Papa, Differential evolution with estimation of distribution for worst-case scenario optimization, *Mathematics*, ISSN 2227-7390, 2021, vol. 9, pp. 2137-1-2137-22, doi: 10.3390/math9172137.

9. Marko Pavlin, Franc Novak, Gregor Papa, Low power contactless bioimpedance sensor for monitoring breathing activity, *Sensors*, ISSN 1424-8220, 2021, vol. 21, pp. 2081-1-2081-14, doi: 10.3390/s21062081.

10. Tome Eftimov, Peter Korošec, Deep statistical comparison for multi-objective stochastic optimization algorithm, *Swarm and evolutionary computation*, ISSN 2210-6502, 2021, vol. 61, pp. 100837-1-100837-16, doi: 10.1016/j.swevo.2020.100837.

Awards and Appointments

1. Carola Doerr dr. Tome Eftimov and Anja Janković received the Best Paper Award at EvoApps 2021 as part of EvoStar: EvoApplications: Towards Feature-Based Performance Regression/Using Trajectory Data (http://www.evostar.org/2021/awards/)

2. Dr Tome Eftimov, dr. Dragi Kocev, Gorjan Popovski, dr Matej Petković in prof. dr Barbara Koroušić Seljak received the ARRS Award Excellent in Science 2021. They received the award in the field of interdisciplinary research with the title of the article: The impact of the COVID-19 pandemic on eating habits.

Organization of conferences, congresses and meetings

1. Online workshop TETRAMAX: Keras and deep learning through examples, Ljubljana, 14. 1. 2021
2. Online workshop TETRAMAX: "Tensorflow: use beyond deep learning", Ljubljana 27. 1. 2021
3. Online workshop AI & Food and Nutrition as part of the conference Applied Machine Learning Days 2021 (AMLD 2021), Ecublens, Switzerland, 26.–30. 3. 2021
4. Online workshop TETRAMAX: »Introduction to Android programming with Kotlin«, Ljubljana 21. 4. 2021
5. Online workshop TETRAMAX: "Creating location services in Android system", Ljubljana 5. 5. 2021
6. Online workshop TETRAMAX: "Identifying quality improvements in industrial optimization", Ljubljana, 25. 5. 2021
7. 38th Slovenian online workshop "Algorithms by Nature Models", Maribor, 28. 5. 2021
8. Online workshop REPL4OPT: Representation Learning meets Meta-heuristic optimization as part of the conference IEEE CEC 2021, Krakow, Poland, 28. 6.–1. 7. 2021
9. Online workshop Good Benchmarking Practices for Evolutionary Computation Benchmarking as part of the conference IEEE CEC-2021, Krakow, Poland, 28. 6.–1. 7. 2021
10. Online workshop Good Benchmarking Practices for Evolutionary Computation Benchmarking as part of the conference GECCO-2021, Lille, France, 10.–14. 7. 2021
11. Performance Assessment of Swarm Intelligence Algorithms as part of 2021 International Conference on Swarm Intelligence (ICSI 2021), Qingdao, China, 17.–21. 7. 2021
12. Online presentation workshop TETRAMAX: ICT solutions for healthy and active aging, 28. 9. 2021
13. 39th Slovenian online workshop "Algorithms by Nature Models", Ljubljana, 1. 10. 2021
14. Online educational workshop TETRAMAX: Design of hardware and embedded systems with FPGA circuits, Ljubljana, 20. 10. 2021
15. Online educational workshop TETRAMAX: Artificial neural networks in practice, Ljubljana, 3. 11. 2021
16. Online educational workshop: Linking Food, Nutrition and Biomedical Data for Trustworthy AI in Predictive Healthcare, Ljubljana, 17. 11. 2021

INTERNATIONAL PROJECTS

1. EFSA - CAFETERIA; Support of Automating Some Specific Steps of Systematic Review Process Using Artifical Intelligence
    Prof. Barbara Koroušić Seljak
    European Food Safety Authority - Efsa
2. H2020 - TRUE; Transition Paths to Sustainable Legume based Systems in Europe
    Dr. Bojan Blažica
    European Commission
3. H2020 - TomRes; A Novel and Integrated Approach to increase Multiple and Combined Stress Tolerance in Plants Using Tomato as a Model
    Dr. Bojan Blažica
    European Commission
4. H2020 - TETRAMAX; TEchnology TRAnsfer via Multinational Application eXperiments
    Dr. Marina Santo Zarnik
    European Commission
5. H2020 - SAAM; Supporting Active Ageing through Multimodal Coaching
    Prof. Barbara Koroušić Seljak
    European Commission
6. H2020 - FNS-Cloud; Food Nutrition Security Cloud
    Prof. Barbara Koroušić Seljak
    European Commission
7. H2020 - METROFOOD-PP; METROFOOD-RI Preparatory Phase Project
    Prof. Barbara Koroušić Seljak
    European Commission
8. H2020 - iRel40; Intelligent Reliability 4.0
    Prof. Gregor Papa
    European Commission
9. H2020 - InSecTT; Intelligent Secure Trustable Things
    Dr. Drago Torkar
    European Commission
10. H2020 - ATHENA; Implementing Gender Equality Plans to Unlock Research Potential of RPOs and RFOs in Europe
    Dr. Vida Vukašinović
    European Commission

11. H2020 - COMFOCUS; Communities on Food Consumer Science
    Prof. Barbara Koroušić Seljak
    European Commission
12. H2020 - DAIS; Distributed Artificial Intelligent Systems
    Prof. Gregor Papa
    European Commission

RESEARCH PROGRAMME

1. Computer Structures and Systems
   Prof. Gregor Papa

R&D GRANTS AND CONTRACTS

1. Context - aware on-device approximate computing
   Dr. Bojan Blažica
2. Quality, Safety and Authenticity of INsect PROtein-Based Food and Feed Products
   Prof. Barbara Koroušić Seljak
3. Toponomastical heritage of Primorska Region
   Asst. Prof. Jurij Šilc
4. Social Innovation for Integrated health CARE of ageing population in ADRION Regions-SI4CARE
   Dr. Bojan Blažica
   The Emillia-Romagna Region
5. Support for Strategic Research and Innovation Partnerships (SRIP) in priority areas of

Smart Specialization
Prof. Gregor Papa
Ministry of Economic Development and Technology
6. Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF)
   Dr. Marina Santo Zarnik
   Ministry of Economic Development and Technology
7. School pot: Continuous upgrade of the web portal „Šolski lonec" to support the implementation of the national dietary guidelines in educational institutions and the transfer of skills in using e-tools for planning quality school menus into practice
   Prof. Barbara Koroušić Seljak
   Ministry of Health
8. Innovative solutions for informed choices: A tool to encourage healthier choices by supporting consumers to monitor and evaluate food composition data
   Dr. Bojan Blažica
   Ministry of Health
9. Supporting residents to reduce the risk of alcohol use through a mobile app
   Dr. Bojan Blažica
   Ministry of Health
10. OPKP: Upgrade of the Open platform for clinical Nutrition (OPKP) with respect to the national dietary guidelines and state-of-the-art ICT
    Prof. Barbara Koroušić Seljak
    Ministry of Health
11. CROSSING - Crossing Borders and Scales - An Interdisciplinary Approach
    Prof. Gregor Papa
    Helmholtz-Zentrum Dresden-Rossendorf E.v.
12. Mr-Bec: Modern approaches for Benchmarking in Evolutionary Computation
    Dr. Tome Eftimov
    Slovenian Research Agency

STAFF

Researchers
1. Asst. Prof. Anton Biasizzo
2. Dr. Bojan Blažica
3. Dr. Tome Eftimov
4. Prof. Peter Korošec
5. Prof. Barbara Koroušić Seljak
6. **Prof. Gregor Papa, Head**
7. Asst. Prof. Veljko Pejović*
8. Dr. Marina Santo Zarnik
9. *Asst. Prof. Jurij Šilc, retired 01.08.21*
10. Dr. Drago Torkar
11. Dr. Vida Vukašinović
Postdoctoral associate
12. Dr. Marko Pavlin*
Postgraduates
13. Margarita Antoniou, M. Sc.
14. Rok Hribar, B. Sc.

15. Gordana Ispirova, B. Sc.
16. Gašper Petelin, B. Sc.
17. *Gorjan Popovski, M. Sc., left 20.03.21*
18. Urban Škvorc, B. Sc.
19. Eva Valenčič, B. Sc.
20. Jure Vreča, B. Sc.
Technical officers
21. Robert Modic, B. Sc.
22. Peter Novak, B. Sc.
23. Matevž Ogrinc, B. Sc.
Technical and administrative staff
24. Jolanda Jakofčič
25. Andraž Simčič
26. Andreja Vlašič, B. Sc.

Note:
* part-time JSI member

BIBLIOGRAPHY

ORIGINAL ARTICLE

1. Tome Eftimov, Bibek Paudel, Gorjan Popovski, Dragi Kocev, "A framework for evaluating personalized ranking systems by fusing different evaluation measures", *Big data research*, 2021, **25**, 100211.
2. Tamara Jakovljević, Milica M. Janković, Andrej M. Savić, Ivan Soldatović, Gordana Čolić, Tadeja Jere Jakulin, Gregor Papa, VanjaKović, "The relation between physiological parameters and colour modificatons in text background and overlay during reading in children with and without dyslexia", *Brain sciences*, 2021, **11**, 5, 539.
3. Nathan Matusheski *et al.* (13 authors), "Diets, nutrients, genes and the microbiome: Recent advances in personalised nutrition", *British journal of nutrition*, 2021, **126**, 10, 1489-1497.
4. Timotej Knez, Octavian-Mihai Machidon, Veljko Pejović, "Self-adaptive approximate mobile deep learning", *Electronics*, 2021, **10**, 23, 2958.
5. Esther Molina-Montes *et al.* (19 authors), "Impact of COVID-19 confinement on eating behaviours across 16 European countries: the COVIDiet cross-national study", *Food quality and preference*, 2021, **93**, 104231.

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7. Gjorgji Noveski, Tome Eftimov, Kostadin Mishev, Monika Simjanoska, "Data-driven intelligence system for general recommendations of deep learning architectures", *IEEE access*, 2021, **9**, 148710-148720.
8. Anton Biasizzo, Barbara Koroušić-Seljak, Eva Valenčič, Marko Pavlin, Marina Santo-Zarnik, Bojan Blažica, Damian O'Kelly, Gregor Papa, "An open-source approach to solving the problem of accurate food-intake monitoring", *IEEE access*, 2021, **9**, 162835-162846.
9. Abhinav Mehrotra, Veljko Pejović, Mirco Musolesi, "FutureWare: designing a middleware for anticipatory mobile computing", *IEEE transactions on software engineering*, 2021, **47**, 10, 2107-2124.
10. Veljko Pejović, Tilen Matkovič, Mojca Ciglarič, "Wireless ranging for contactless cognitive load inference in ubiquitous computing", *International journal of human-computer interaction*, 2021, **37**, 19, 1849-1873.

11. Tadej Krivec, Gregor Papa, Juš Kocijan, "Simulation of variational Gaussian process NARX models with GPGPU", *ISA transactions*, 2021, **109**, 141-151.

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18. Maša Hribar, Hristo Hristov, Živa Lavriša, Barbara Koroušić-Seljak, Matej Gregorič, Urška Blaznik, Katja Žmitek, Igor Pravst, "Vitamin D intake in slovenian adolescents, adults, and the elderly population", *Nutrients*, 2021, **13**, 10, 3528.

19. Barbara Koroušić-Seljak *et al.* (14 authors), "Inadequate intake of dietary fibre in adolescents, adults, and elderlies: results of Slovenian representative Si.Menu study", *Nutrients*, 2021, **13**, 11, 3826.

20. Igor Pravst *et al.* (14 authors), "Dietary intake of folate and assessment of the folate deficiency prevalence in Slovenia using serum biomarkers", *Nutrients*, 2021, **13**, 11, 3860.

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23. Marko Pavlin, Franc Novak, Gregor Papa, "Low power contactless bioimpedance sensor for monitoring breathing activity", *Sensors*, 2021, **21**, 6, 2081.

24. Tamara Jakovljević, Milica Janković, Andrej Savić, Ivan Soldatović, Petar Todorović, Tadeja Jere Jakulin, Gregor Papa, VanjaKović, "The sensor hub for detecting the developmental characteristics in reading in children on a white vs. colored background/colored overlays", *Sensors*, 2021, **21**, 2, 406.

25. Tome Eftimov, Peter Korošec, "Deep statistical comparison for multi-objective stochastic optimization algorithm", *Swarm and evolutionary computation*, 2021, **61**, 100837.

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Published Conference Contribution

1. Gordana Ispirova, Tome Eftimov, Barbara Koroušić-Seljak, "Exploring knowledge domain bias on a prediction task for food and nutrition data", V: *2020 IEEE International Conference on Big Data (Big Data), Atlanta, Georgia, USA, 10-13 December 2020*, IEEE, 2021, 3563-3572.

2. Jure Vreča, Iva Ivanov, Gregor Papa, Anton Biasizzo, "Detecting network intrusion using binarized neural networks", In: *2021 IEEE 7th World Forum on Internet of Things (WF-IoT), 14 June-31 July 2021, New Orleans, LA, USA*, IEEE, 2021, 622-627.

3. Urban Škvorc, Tome Eftimov, Peter Korošec, "The effect of sampling methods on the invariance to function transformations when using exploratory landscape analysis", In: *2021 IEEE Congress on Evolutionary Computation (CEC), June 28th-July 1st 2021, Kraków, Poland*, IEEE, 2021, 1139-1146.

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6. Andraž Krašovec, Gianmarco Baldini, Veljko Pejović, "Opposing data exploitation: behaviour biometrics for privacy-preserving authentication in IoT environments", In: *ARES 2021, 16th International Conference on Availability, Reliability and Security, Vienna, Austria, August 17-20, 2021*, Proceedings, ACM, 2021.

7. Gjorgjina Cenikj, Tome Eftimov, Barbara Koroušić-Seljak, "SAFFRON: tranSfer leArning For Food-Disease RelatiOn extractioN", In: *Twentieth Workshop Biomedical Language Processing (BioNLP), June 11th 2021*, Proceedings, ACL Anthology, 2021, 30-40.

8. Gordana Ispirova, Gorjan Popovski, Eva Valenčič, Nina Hadži-Kotarova, Tome Eftimov, Barbara Koroušić-Seljak, "Food data normalization using lexical and semantic similarities heuristics", V: *BIOSTEC 2020, 13th International Joint Conference on Biomedical Engineering Systems and Technologies, February 24-26 2020, Valletta, Malta*, revised selected papers, (Communications in Computer and Information Science **1400**), Springer, 2021, 468-485.

9. Angela Kralevska, Marija Velichkovska, Viktor Cicimov, Tome Eftimov, Monika Simjanoska, "Finding potential inhibitors of COVID-19", In: *BIOSTEC 2021, 14h International Joint Conference on Biomedical Engineering Systems and Technologies, February 11-13*, Proceedings, volume 3 Bioinformatics, SciTePress, 2021, 110-117.

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11. Octavian-Mihai Machidon, Davor Sluga, Veljko Pejović, "Queen Jane approximately: enabling efficient neural network inference with context-adaptivity", In: *EuroMLSys 21, 1st Workshop on Machine Learning and Systems, April 2021*, Proceedings, ACM, 2021, 48-54.

12. Hao Wang, Carlos Ignacio Hernández Castellanos, Tome Eftimov, "On statistical analysis of MOEAs with multiple performance indicators", In: *EMO 2021, 11th International Conference Evolutionary multi-criterion optimization, Shenzhen, China, March 28-31, 2021*, Proceedings, (Lecture notes in computer science **12654**), Springer, 2021, 26-37.

13. Ana Kostovska, Diederick Vermetten, Carola Doerr, Sašo Džeroski, Pance Panov, Tome Eftimov, "OPTION: optimization algorithm benchmarking ontology", In: *GECCO '21, Genetic and Evolutionary Computation Conference, July 10 - 14, 2021, Lille, France*, Proceedings, ACM, 2021, 239-240.

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16. Gregor Papa, "Applications of dynamic parameter control in evolutionary computation", In: *GECCO '21, Genetic and Evolutionary Computation Conference, July 10 - 14, 2021, Lille, France*, Proceedings, ACM, 2021, 1064-1088.

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26. Andrej Kastrin, Rok Hribar, Gregor Papa, Janez Povh, "Bibliographic data clustering based on symmetric non-negative matrix tri-factorization", In: *SOR '21, 16th International Symposium on Operational Research in Slovenia, September 22-24, 2021*, Proceedings, Slovenian Society Informatika, Section for Operational Research, 2021, 194-199.

27. Emir Hasanbegović, Veljko Pejović, "Uncovering personal and context-dependent display preferences in mobile newsreader app", In: *UMAP '21, 29th ACM Conference on User Modeling, Adaptation and Personalization, June 21-25 2020, Utrecht, Netherlands*, Proceedings, ACM, 2021, 5-13.

Independent Component Part or a Chapter in a Monograph

1. Rok Hribar, Gašper Petelin, Jurij Šilc, Gregor Papa, Vida Vukašinović, "Memetic algorithm and evolutionary operators for multi-objective matrix tri-factorization problem", In: *Heuristics for optimization and learning*, (Studies in computational intelligence **906**), Springer, 2021, 286-298.

2. Margarita Antoniou, Peter Korošec, "Multilevel Optimisation", In: *Optimization under uncertainty with applications to aerospace engineering*, Springer, 2021, 307-331.

3. Margarita Antoniou, Rok Hribar, Gregor Papa, "Parameter control in evolutionary optimisation", In: *Optimization under uncertainty with applications to aerospace engineering*, Springer, 2021, 357-385.

Scientific Monograph

1. Miha Kosi, Matjaž Bizjak, Miha Seručnik, Jurij Šilc, *Historična topografija Kranjske (do 1500)*, (Slovenska historična topografija **1**), 2. e-izdaja, Založba ZRC, 2021.

Theses and Mentoring

1. Tamara Jakovljević, *The sensor hub for detection of the relation between physiological parameters and colour modifications in text background and overlay during reading in children with and without dyslexia:* doctoral dissertation, Ljubljana, 2021 (mentor Gregor Papa; co-mentor Tadeja Jere Jakulin).

2. Simon Mezgec, *Food and drink image detection and recognition using deep convolutional neural networks:* doctoral dissertation, Ljubljana, 2021 (mentor Barbara Koroušič Seljak).

DEPARTMENT OF KNOWLEDGE TECHNOLOGIES E-8

At the Department of Knowledge Technologies we develop artificial intelligence methods and other advanced information technologies that support the acquisition, management, modeling and use of knowledge and data, thus enabling a knowledge-based society. Our research covers many areas of artificial intelligence, such as machine learning and natural language processing, as well as related fields, such as decision support. Our research has five pillars: machine learning, decision support and artificial intelligence, artificial intelligence and science, natural language processing and digital humanities, and knowledge technologies for society. We use the developed knowledge technologies in various fields, from sustainable agriculture to personalized medicine and health, through media, education and the arts, to various industrial sectors such as energy, transport and space research.

Head:
Prof. Sašo Džeroski

In 2021 we were involved in twenty-one national projects and thirteen Horizon 2020 projects, and were the coordinators of two EU projects, EMBEDDIA and IMSyPP. We were also involved in two COST actions, one CEF project, two infrastructure projects, and four industry projects. Finally, we had five young-researcher projects, through which we hosted junior researchers working towards their PhDs.

Machine Learning. In this area we focused on *multi-target prediction,* developing various methods addressing different machine-learning tasks. First, we designed novel methods for learning oblique decision trees for simple supervised tasks such as classification and regression, as well as for more complex supervised tasks of structured output prediction such as multi-label classification, hierarchical multi-label classification and multi-target regression. Second, we extended these methods towards semi-supervised learning for both simple and complex learning tasks (such as structured output prediction). Next, we developed a methodology for fusing different evaluation measures in the context of recommender systems. Finally, we performed a study to analyze and explain the performance of multi-label classification methods with data set properties.

In the field of machine learning we also addressed the topic of *representation learning* where we developed data mining methods for the analysis of heterogeneous data and used them in several application domains. A top scientific achievement is the publication of the scientific monograph entitled *Representation Learning: Propositionalization and Embeddings*, written by N. Lavrač, V. Podpečan and M. Robnik-Šikonja, Springer, 2021, 163 pages. The monograph presents several original machine learning methods for representation learning (RSD, Wordification, PropStar and PropDRM), methods of transforming semantically tagged data (SDM-Aleph and NetSDM) and methods for automated heterogeneous information network transformation (TEHmINe and HIN-MINE). In addition to the original algorithms, the monograph provides a comprehensive overview of the research field of representation learning, achieved through a common terminology and a unifying framework that enabled the authors to establish a unifying description of the representation learning techniques for classical machine learning and modern deep neural networks. We developed a novel Deep Node Ranking (DNR) algorithm, published in the International Journal of Intelligent Systems. It allows for neuro-symbolic learning of representations and classification of network nodes, which was applied to the problem of an efficient functional annotation of unknown proteins and the perception of bots on social networks. We developed a new approach for the node regression analysis based on the transfer learning approach and used for the analysis of activation spreading, published in the Complex Systems journal.

Decision Support and Artificial Intelligence. In the area of *decision support*, our long-term goal is to develop methods and techniques of decision modeling, support them with software and integrate them with data mining systems. In 2021 we were developing a new generation of software for the construction and use of decision models in accordance with the DEX method. In addition to a more modern technological design, supporting the method in different environments (Web, Java, .NET, R, Python), the DEX method is being extended according to the proposals and developments from the previous years: integration of qualitative and quantitative elements, relational modeling, advanced analyses of alternatives. The web version of the software, Dex2Web, was described in an award-winning paper. In the Springer's book *Euro Working Group on DSS: A Tour of the DSS Developments Over the Last 30 Years*,
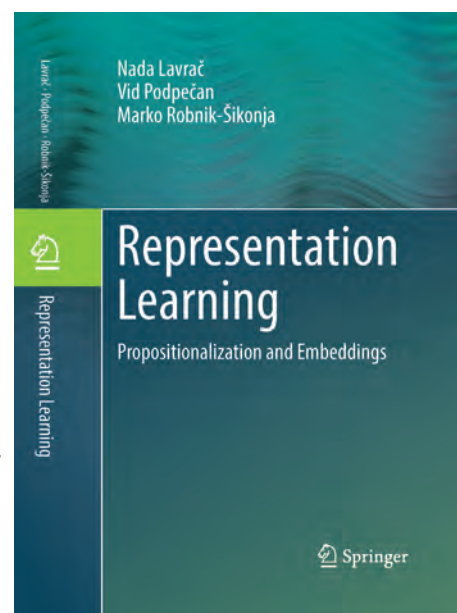

Figure 1: Cover page of the scientific monograph *Representation Learning: Propositionalization and Embeddings, by N. Lavrač, V. Podpečan and M. Robnik-Šikonja, published by Springer 2021.*

which summarizes the last thirty years of development of the field of decision-support systems, we contributed a chapter on our experience in building decision models and their combination with machine learning methods in demanding decision situations. In the context of developing decision support systems for agriculture, we developed the DEXiWare tool, which is intended for an efficient integration of modules that make up decision support systems based on multicriteria decision models. The tool is intended for DSS researchers and developers, and its general description is given on the DEXiWare website (http://dexiware.ijs.si/).

In the area of *explainable artificial intelligence,* we developed and evaluated methods for variable importance estimation and feature ranking in several contexts. This includes novel methods for feature ranking in multi-class and multi-label classification, based on low-dimensional manifold embeddings of the input and output spaces and the relief method. Similarly, this includes new approaches for unsupervised feature ranking based on the predictive clustering framework as well as the relief family of methods, on the one hand, and based on attribute networks, on the other hand. Moreover, we developed and evaluated a method for comparing ordered lists (named the fuzzy Jaccard index), which can be applied in a range of contexts, including feature rankings, information retrieval, etc.

Department members participated in the shared task of COVID-19 fake-news detection in the scope of the workshop "CONSTRAINT 2021 Fighting an Infodemic: COVID-19" collocated with AAAI 2021. The goal was to decide for a given document whether it included false claims related to COVID-19. Our approach was ranked among the top 5% of the teams, and our solution was within 1.5% of the best results.

Artificial Intelligence for Science. In this area, we continued working on *semantic technologies* to support the process of data analysis in the spirit of *open scienc*e. In addition, we started collaborating on the development of ontological resources for the domain of optimization. In particular, the IMPERATRIX project aims at improving the repeatability of experiments and reusability of research outputs in complex data analysis. Within it, we worked on further development of ontological descriptions of machine learning algorithms, development of a web-based system for querying multi-label classification datasets and experiments. We extended the OntoDM-core ontology with a module for representing machine learning algorithms and included a more detailed representation of algorithms, including terms such as hyperparameter, optimization problem, complexity function, etc. The developed ontology module will be used as the backbone of a repository and knowledge base for storing semantic annotations of algorithms and for assisting algorithm developers and domain experts.

We developed the optimization algorithm benchmarking ontology (OPTION) to support benchmarking of algorithms in the domain of optimization. Our ontology provides the vocabulary needed for semantic annotation of the core entities involved in the benchmarking process, such as algorithms, problems, and evaluation measures. It also provides means for automated data integration, improved interoperability, powerful querying capabilities and reasoning, thereby enriching the value of the benchmark data. We demonstrated the utility of OPTION by annotating and querying a corpus of benchmark performance data from the BBOB workshop data, a use case that can be easily extended to cover other benchmarking data collections.

In the field of *computational scientific discovery*, a key area of using artificial intelligence for science, our research concentrated within the SESAME project – Automating the Synthesis and Analysis of Scientific Models. Here we proposed the use of probabilistic grammars to represent domain knowledge in equation discovery. We also applied the approach of automated process-based modeling of dynamic systems to model urban runoff as well as design stormwater control measures.

In the related field of *computational creativity*, we developed new methods for the creative generation of a natural language text based on a general architecture for computational creativity. We applied these methods to the domain of weather reports. We also proposed a novel method for an automated generation of scientific questions and integrated it into our RoboCHAIR system.

We also extensively used *machine learning for science*, considering scientific data from different domains, resulting in publications in both computer science and application domain literature. In the area of life sciences, medicine and pharmacology, we performed a virtual compound screening, looking for drugs that would help reverse lung fibrosis, within the INTERREG V-A Slovenia-Italy project TRAIN: Big Data and Disease Models: A Cross-Border Platform for Validated Biotech Industry Kits. Within three national projects in this area, we develop the infrastructure, e.g., for bioinformatics (RI-SI ELIXIR), and use it for problems relating to life sciences, as well as considering environmental exposure and human health. The latter is the topic of the "NEURODYS project – Neuropsychological dysfunctions caused by low level exposure to selected environmental pollutants in susceptible population", which looks at the effects of exposure to mercury on the health of mothers and children.

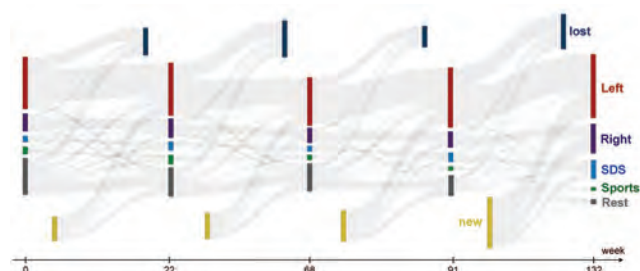*Figure 2: A Sankey diagram showing community membership transitions at five timepoints during the 2018–2020 period. There are four major communities identified: Left (red), Right (violet), SDS (blue), and Sports (green). The remaining, typically smaller, communities are denoted as Rest. Note that at each timepoint, there are new Twitter users joining the retweet networks, and lost users leaving the networks.*

Within the project "Restoration of moldy canvas paintings: improvement or deterioration?", we study the damage to paintings caused by fungi, and have analyzed the relation between the properties of paintings and such damage.

Language Technologies and Digital Humanities. In these areas, we address the issues of natural language processing and understanding, text and network analytics, open-access language resources, and digital humanities. In the field of *natural language processing and understanding*, we continued our work on the European project EMBEDDIA (Cross-Lingual Embeddings for Less-Represented Languages in European News Media) that we coordinate. The project seeks to solve many problems for the news media industry concerning the analysis of news and comments, especially by leveraging innovations in the use of cross-lingual embeddings, coupled with deep neural networks, allowing the existing monolingual resources to be used across languages. In 2021 the main event demonstrating the results to the research community was a hackashop on news media content analysis and automated report generation, a hackathon/workshop that we organized in the scope of the conference of the European Association of Computational Linguistics (EACL) where 24 researchers from academia and industry took part. The main event targeting industry professionals was the conference on "EMBEDDIA AI tools for the media industry" in December 2021 where tools were demonstrated to more than 80 participants from media companies and research institutions from around Europe. We also co-organized a shared task on named-entity recognition in Slavic languages and proposed a novel approach to named-entity recognition.

The majority of our deep-neural-network-based methods use transfer learning based on language-model pre-training to allow better performance with less labelled training data. We have recently leveraged this approach to develop novel methods for text-readability assessment. We also developed a neural keyword extraction system known as TNT-KID, extended it to achieve better recall, and the system is now being tested for real-life deployment by Estonia's largest news media house. For the same media house we also presented an approach for retrieving interesting news from another country, while we also worked on topic categorization using the data from the Finnish press agency STT.

Figure 3: Main solutions integrated into the EMBEDDIA media assistant (https://embeddia.texta.ee/)

We started work on the EU project MaCoCu (Massive Collection and Curation of Monolingual and Bilingual Data: Focus on Under-Resourced Languages) by setting up a web crawling infrastructure and performing the first iteration of the crawls of 12 targeted top-level domains. The web crawls will be used for constructing large monolingual text collections for building pre-trained language models and for extracting translations for improving machine-translation models. We have started our work for further enrichment of the crawled data by setting up a new schema and dataset for web-based genre identification (http://hdl.handle.net/11356/1467).

We also continued our work aimed at understanding and optimizing machine learning methods for NLP. We developed explanation techniques for neural classifiers by extending SHAP explanations, or by using a self-attention analysis. We also developed an autoML approach, autoBOT, in which we use an evolutionary algorithm to jointly optimize various sparse and dense representations for a given text classification task, and applied subgroup discovery methods for understanding news sentiment.

In the scope of the project CANDAS (Computer-assisted multilingual news discourse analysis with contextual embeddings), we adapted our contextual-embeddings-based methods for investigating different viewpoints across news sources reporting on the topic of LGBTIQ+ and COVID-19, and worked on semi-automated metaphor extraction. In the TermFrame (Terminology and Knowledge Frames across Languages) project, we contributed to the development of a multi-modal knowledge base for karstology and proposed a method for word-embeddings-based terminology alignment.

We also developed new methods for the fundamental NLP task of semantic parsing, using two approaches: one based on incremental parsing using vector-space models, designed to be suitable for dialogue processing, and the other based on large pre-trained neural models using

The EMBEDDIA project organized two events for promoting the resources and solutions, as well as tools that are grouped under the title "EMBEDDIA Media Assistant". The hackashop on news media content analysis and report generation was a hackathon/workshop collocated with EACL 2021 with 24 research participants, while the conference "EMBEDDIA AI tools for the media industry" was attended by more than 80 participants from the media companies and research institutions from around Europe.

simplified intermediate representations, which achieved new state-of-the-art results for parsing a natural language text to SQL queries for a database search. We also developed methods for understanding the structure of dialogue and interaction in large groups, based on the neural NLP and social network analysis, to understand the nature of explanation, decision-making and influence in large organizations.

One line of our applied research focused on COVID-19. We developed a method for COVID-19 fake-news detection, using a neural stacking approach. Next, we developed an online system for prioritization of COVID-19-related literature via unsupervised keyphrase extraction and document representation learning. In addition, we participated

in a shared task on multi-label classification of COVID-19-related articles. Another research direction was the assessment of cognitive impairment. We developed multimodal methods for Alzheimer's diagnosis, using temporal integration of text, interaction and acoustic features based on spontaneous speech.

In the field of *text and network analytics*, our research approach is to combine methods of text mining, natural language processing, network analysis and topic detection to reveal and highlight underlying characteristics in different domains. The main sources of data that we analyze are social media (Twitter, Facebook, YouTube). We are coordinating an EU project called IMSyPP (Innovative Monitoring Systems and Prevention Policies of Online Hate Speech) with the goal to develop models for automated hate-speech detection and tracking. We constructed and analyzed the Slovenian retweet network in the period 2018–2020. The community-detection results show an evolution of communities through time with an increasing polarization between the left- and right-wing super communities. The topics detected show that politics and ideology prevail, and that they also attract the largest fraction of hateful tweets. An analysis of the Italian YouTube comments reveals a similar distribution of hate-speech classes as on Slovenian Twitter. However, there was no clear or significant relation between the levels of hate speech and misinformation.

In the scope of the project Formica 2 (Quantitative and qualitative analysis of the unregulated corporate financial reporting) we compared various methods for forward-looking sentence extraction from annual reports, and contributed to the FinSim-2 task on the financial concept classification.

We continued work on the Slovenian-Flemish bilateral basic research project LiLaH (Linguistic landscape of hate speech on social media), inside which we published English, Slovenian and Croatian datasets of Facebook comments, manually-annotated for hate speech together with the corresponding prediction models (https://huggingface.co/classla). We also released state-of-the-art transformer models for Croatian, Bosnian, Montenegrin and Serbian BERTić (https://huggingface.co/classla/bcms-bertic) and the commonsense reasoning benchmark for Croatian COPA-HR (http://hdl.handle.net/11356/1404). Related to this project, we also participated in publishing the Croatian psycholinguistic database to be used for analyzing

Figure 4: A schematic illustration of the training regime for cross-lingual offensive speech detection experiments.

implicit and covert hate speech. Finally, we organized the shared task on multilingual text normalization, MultiLexNorm, and participated in the shared task, our system being ranked second best. Related to the processing of non-standard language, we published a journal article on collaborative development of the research infrastructure for processing non-standard language in Slovenian, Croatian and Serbian.

Cross-lingual embeddings can be used to transfer machine learning models between languages, thereby compensating for insufficient data in less-resourced languages. We used cross-lingual word embeddings to transfer machine-learning prediction models for Twitter sentiment between 13 languages. Our experiments show that the transfer of models between similar languages is sensible, while dataset expansion does not increase the predictive performance. Similarly, we addressed the task of offensive language detection in zero-shot and few-shot learning where no or only few examples of training data in the target language are available; this is now being tested for real-world deployment by the Croatian 24sata news portal. Finally, the transfer-learning approach was applied for the task of diachronic semantic change detection and to explore scientific discourse on the topic of ecosystem services.

Sašo Džeroski and Marko Debeljak gave invited lectures at the 6th Web Conference on New Technologies in Agriculture, on 9 December 2021, presenting opportunities for and examples of using artificial-intelligence methods in agriculture.

In the field of *open-access language resources,* we lead CLARIN.SI, the Slovenian national node of the European CLARIN ERIC research infrastructure, which provides easy publication and sustainable access to digital language data for scholars in the humanities and social sciences and other disciplines that use or produce language resources. CLARIN.SI maintains the CTS-certified CLARIN.SI repository, concordancers and other Web services, and supports the creation-language resources and promotion of digital linguistics.

CLARIN.SI was a partner in the CLARIN ERIC-funded project ParlaMint "Towards Comparable Parliamentary Corpora" that we successfully concluded in 2021. We led the compilation of the 500-million-word ParlaMint corpus, which contains linguistically annotated parliamentary proceedings of 17 European countries in 16 languages, and was published in the CLARIN.SI repository under the CC BY license [http://hdl.handle.net/11356/1405, http://hdl.handle.net/11356/1388]. CLARIN.SI participated in the European project "RDA Node Slovenia" lead by the Slovenian node of the CESSDA research infrastructure. We lead the Working Group on the coordination of the Slovenian
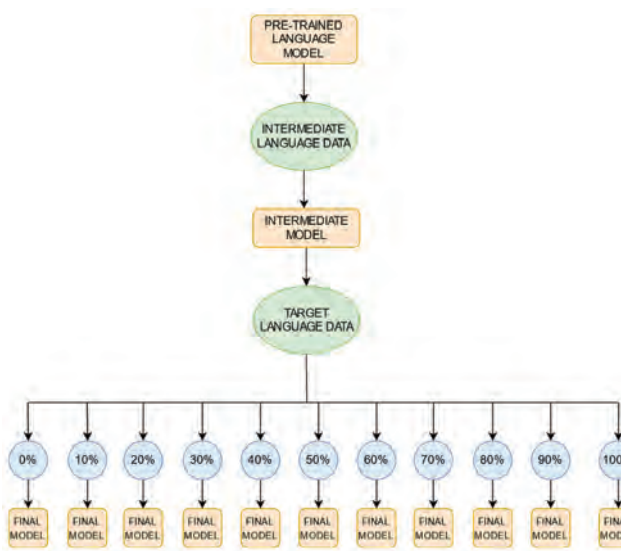
repositories of research data, where we produced a survey-based quantitative and qualitative analysis of 13 such repositories, with a focus on certification and FAIR principles.

In the scope of the project "Development of Slovenian in a Digital Environment", financed by the Slovenian Ministry of Culture and with partners from 12 institutions, the JSI has been developing methods for terminology extraction and semantic change detection. In this project, CLARIN.SI is tasked with making all the resources produced within the project to be archived and made openly available in the CLARIN.SI repository. CLARIN.SI also

offers its WebAnno platform for manual corpus annotation and help in annotation campaigns, as well as giving guidelines for the use of standards and best practices in encoding and annotation of the project's language resources. As a case in point, we helped with the annotation of the Corpus of term-annotated texts RSDO5, which was then published in the CLARIN.SI repository [http://hdl.handle.net/11356/1400]. In the scope of the project,

The PathFinder decision-support system, developed within the H2020 project TRUE, was officially launched on 30 September 2021. A recording of the launch can be found at: https://bit.ly/33p9PSY

we contributed new versions of three Slovenian reference corpora, i.e., the Training corpus ssj500k 2.3. [http://hdl.handle.net/11356/1434], the Spoken corpus Gos 1.1. [http://hdl.handle.net/11356/1438] and Spoken corpus Gos VideoLectures 4.2 (transcription) [http://hdl.handle.net/11356/1444]. We also released three new versions of the Slovenian linguistic annotation pipeline CLASSLA [https://pypi.org/project/classla/].

We encoded and linguistically annotated several corpora, which were compiled at ZRC SAZU: the Corpus of 1968 Slovenian literature Maj68 [http://hdl.handle.net/11356/1430], the Corpus of Slovenian school texts [http://hdl.handle.net/11356/1413], and the corpus of older Slovenian narrative prose PriLit [http://hdl.handle.net/11356/1319].

As part of the work of the CLARIN.SI and CLADA-BG Knowledge Centre for South Slavic languages (CLASSLA) we published the Comparable corpora of South-Slavic Wikipedias CLASSLA-Wikipedia, the Corpus of Croatian news portals ENGRI (2014–2018) [http://hdl.handle.net/11356/1416], the Montenegrin web corpus meWaC [http://hdl.handle.net/11356/1429], the Text collection for training the BERTić transformer model BERTić-data [http://hdl.handle.net/11356/1426], the Croatian corpus of non-professional written language by typical speakers and speakers with language disorders RAPUT 1.0 [http://hdl.handle.net/11356/1435], the Corpus of Serbian forms of address [http://hdl.handle.net/11356/1422], and a new version of the CLASSLA-StanfordNLP model for morphosyntactic annotation of standard Macedonian [http://hdl.handle.net/11356/1395] and standard Slovenian [http://hdl.handle.net/11356/1392], which can be used with our CLASSLA fork of the well-known Stanza annotation tool-chain for text annotation. We also released the first open model for automatic speech recognition of Croatian [https://huggingface.co/classla/wav2vec2-xls-r-parlaspeech-hr].

CLARIN.SI was, in 2020, a co-organizer of the biennial Conference on Language Technologies and Digital Humanities. In 2021 we edited a special issue of the Slovenščina 2.0 journal, which contains a selection of expanded papers from the proceedings of the conference. At the CLARIN ERIC level, we participated in consolidating and maintaining the CLARIN resource and tool families and contributing to the work of the CLARIN Standards Committee.

We also contribute to the work of the Slovenian Institute for Standardization as the Slovenian representatives in ISO TC37/SC4 (Language and Terminology / Language Resources Management) by reviewing, translating and approving Slovenian standards from this field.

In the field of *digital humanities*, we participate in the COST action "Distant Reading for European Literary History" where we produced the Slovene ELTeC corpus, which contains one hundred novels from the period 1840 to 1920 that were also linguistically annotated. We started work on two new Slovenian basic research projects, both lead by ZRC SAZU, the Scientific Research Center of the Slovenian Academy of Sciences and Arts, namely "Traditional Paremiological Units in Dialogue with Contemporary Use" and "Formant Combinatorics in Slovenian".

Knowledge Technologies and Society. This part of our work concerned the use of knowledge technologies for solving practically relevant problems from many different areas, ranging from agriculture and industry, through medicine and healthcare, to media and education. In the area of *agriculture and environment* we were involved in several projects where we used data-mining and decision-modeling methods to develop predictive and decision models to support a sustainable agricultural development. In addition, in cooperation with the institute INRAE, France, we developed two decision-support systems, based on the use of the DEX method: for suppressing the fruit fly and mitigating fungal infections of the creeping thistle.

As part of the H2020 TRUE project (Transition paths to sustainable legume-based systems in Europe), we successfully completed the development of a decision-support system for assessing and managing the sustainability of agri-food chains – Pathfinder. The system assesses sustainability by integrating the environmental, economic and social pillars of sustainability. It gives an estimate for each pillar of the individual links of the chain, the pillars of the whole chain and the sustainability of the chain as a whole. In addition to evaluation, it also allows the user to do a what-if analysis (bottom-up) and an analysis of possible scenarios (top-down). To communicate with the user, we developed a user-friendly graphical interface. We validated the system on six different agri-food chains. Due to its high reliability (94.7%), it was officially launched for public use at the end of the project (September 2021)

(https://pathfinder.ijs.si/). More detailed descriptions of the Pathfinder system are given in the publicly available project deliverables.

The H2020 TomRes project (A novel and integrated approach to increase multiple and combined stress tolerance in plants using tomato as a model) concluded with the development of a decision-support system, ResourceAmplifier, for the selection of management measures that improve water and nutrient resource efficiency for tomato production. The system also provides an assessment of the impact of tomato production on the environment and the producers' socio-economic situation. The system was developed for tomato production in greenhouses and outdoors. The end user communicates with the ResourceAmplifier system (http://resourceamplifier.ijs.si/) via a user-friendly web-based graphical interface. A more detailed description of the ResourceAmplifier system is given in the publicly available project deliverable.

In the IPM Decisions project (Stepping-up IPM decision support for crop protection), which aims to improve the use of the existing decision support systems (DSSs) in integrated plant protection (IPM), we carried out a systematic cataloging of 80 existing DSSs. The cataloging was performed with the help of the typology of DSSs in the field of plant protection, which we developed for this purpose. The results were given in the project deliverable, and an application is currently being developed that will make it easier for the users to review the collected decision support systems. Based on the results of the analysis of the surveys on user experience of farmers, farm advisors and developers using DSSs in integrated plant protection, we prepared a new questionnaire. Using this questionnaire, we will select the most appropriate measures to improve the user experience and the use of the existing DSSs.

In the H2020 project COCOREADO (Connecting consumers and producers to rebalance farmers' position), we were very active in communicating with potential stakeholders (farms, innovative food chains) from Slovenia who will be involved in the project. The selected stakeholders will participate in the development and verification of the effectiveness of the decision support system in the field of sustainable public procurement in public institutions.

Our activities in the RADIANT project (Realising dynamic value chains for underutilised crops) were also connected to the supply chains. Here we started developing a completely new methodological approach for the analysis of dynamic supply chains in the case of underutilized crops. We plan to develop a decision-support system that would shorten and optimize the supply chain, while helping consumers to meet their demands. The whole system will be based on sustainability criteria. With this, we will enable an optimization of the production conditions of the most locally adapted crops, thus reducing the risk of a decrease in food production due to direct and indirect consequences of the global climate change.

In the area of health and well-being we completed the HeartMan project, under which we developed a computerized system to help patients and doctors in the management of congestive heart failure. We have also successfully finished the SAAM H2020 project (Supporting Active Aging through Multimodal Coaching) where we developed a virtual assistant-coach that supports the aging population living at home. Our work focused on developing the modeling and reasoning components of the coaching system; we prepared the modules for sleep quality, cooking activity, mobility and social activity. All modules were tested in real-life installations within the pilot study. In order to increase the effectiveness of coaching, we also developed a novel method for preference learning based on user feedback as reported for different coaching messages that were received by the users.

Our work for the RESILOC project (Resilient Europe and Societies by Innovating Local Communities), which aims at improving the resilience of local communities, continued with the development of a software tool for assessing and presenting the topics and sentiments of social-media posts that are relevant for studying the resilience to natural disasters. In the frame of the ongoing HECAT project, we developed several disruptive decision-support models included in two web platforms: for human resources management for customs offices and for public employment services. The development of decision models included private employment services as well.

In the area of *knowledge technologies for education* we continued our collaboration with the University of Nova Gorica and JSI Center for Knowledge Transfer in IT. Our activities broadened the scope of target open education applications to also cover management processes, such as identifying knowledge gaps, quality assessment

Sašo Džeroski and Dragi Kocev organized the on-line conference Space and AI, the second edition of the conference on space-related use of artificial intelligence (AI), on 13 September, in conjunction with ECML PKDD 2021, the European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases. With 3 keynotes and 19 contributed presentations, it attracted over 130 participants.
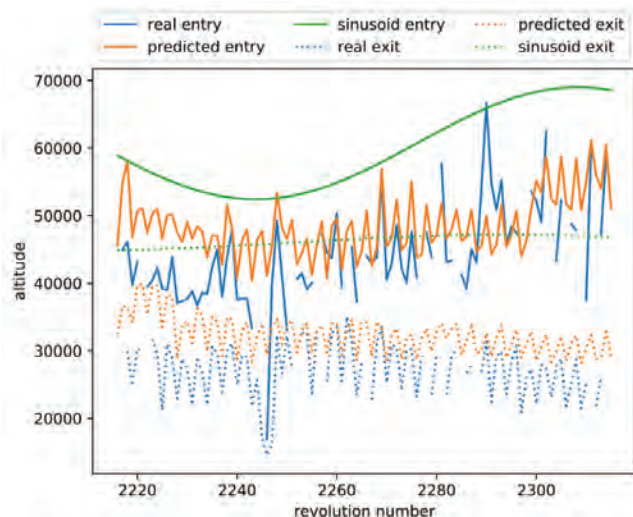
Figure 5: The developed models for predicting the entry and exit altitudes for the INTEGRAL spacecraft allow two more hours per orbit for performing scientific measurements as compared to the currently used sinusoid model.

and shaping strategic policies. We aimed at enhancing the cooperative creation of Open Educational Resources (OERs) for the implementation of Sustainable Development Goals (SDGs). Projects developed in the SDG7-related hubs of the Open Education for the Better World program (OE4BW) devoted to energy, biodiversity and sustainable living were tackled with a focus on the interconnections with other SDGs and processes contributing to closing the knowledge gaps. The resulting guidelines were generalized to provide a further increase in the OERs contribution to the achievement of the SDGs, with a journal paper to be published. We identified open issues to be solved with the applications of data mining. With the colleagues from Germany and Brazil, we are preparing a publication on a novel approach to the development of supportive policies for OERs that was tested within the Leadership in Open Education Master's Program and has proved to be a powerful mechanism for analyzing and creating a roadmap for OERs for organizations and groups.

Finally, we also applied knowledge technologies to problems from *industry*, with a focus on the *space sector*. A cluster of applied projects and research looked at the use of machine learning for Earth observation and space operations. These include the projects "GalaxAI - Machine Learning for Predicting Spacecraft Subsystem Power Consumption", which concerns space operations, and "AiTLAS - AI Prototyping Environment for Earth Observation", which is concerned with Earth observation. We studied the outliers appearing in the telemetry data for the Mars Express spacecraft related to the thermal power consumption. Next, we studied the effect of data frugality and different operation contexts on the predictive performance of the learned models. Finally, we presented a toolbox for an interpretable analysis of the spacecraft telemetry data.

Some outstanding publications in the past year

1. Bohanec, Marko, Vodopija, Aljoša, Luštrek, Mitja, et al. HeartMan DSS: a decision support system for self-management of congestive heart failure. Expert Systems with Applications, 2021, vol. 186, pp. 115688-1-115688-13. ISSN 0957-4174, doi: 10.1016/j.eswa.2021.115688.

2. Brence, Jure, Todorovski, Ljupčo, Džeroski, Sašo. Probabilistic grammars for equation discovery. Knowledge-Based Systems, ISSN 0950-7051, 2021, vol. 224, pp. 107077-1-107077-12, doi: 10.1016/j.knosys.2021.107077.

3. Evkoski, Bojan, Ljubešić, Nikola, Pelicon, Andraž, Mozetič, Igor, Kralj Novak, Petra. Evolution of topics and hate speech in retweet network communities. Applied Network Science, ISSN 2364-8228, 2021, vol. 6, pp. 96-1-96-20, doi: 10.1007/s41109-021-00439-7.

4. Evkoski, Bojan, Mozetič, Igor, Ljubešić, Nikola, Kralj Novak, Petra. Community evolution in retweet networks. PloS ONE, ISSN 1932-6203, 2021, vol. 16, no. 9, pp. e0256175-1-e0256175-21, doi: 10.1371/journal.pone.0256175.

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Organization of conferences, congresses and meetings

1. EACL hackashop on news-media content analysis and automated report generation, 19. 4. 2021 (virtual)
2. 8th BSNLP Workshop on Balto-Slavic Natural Language Processing, 20. 4. 2021 (virtual)
3. VarDial workshop 2021, 20.4.2021 (virtual)
4. VarDial evaluation campaign, 20.4.2021 (virtual)
5. MultiLexNorm shared task, 11.11.2021 (virtual)
6. Space and Artificial Intelligence, 2nd Online Conference, 13. 9. 2021. (virtual)
7. EMBEDDIA Conference: AI Technology for the Media Industry. 8. 12. 2021 (virtual)

Awards and Appointments

1. Tomaž Erjavec: Steven Krauwer Award, Netherlands, CLARIN Annual Conference, CLARIN ERIC, compilation of the multilingual ParlaMint corpus of parliamentary debates
2. Dragi Kocev: Article "COVID-19 pandemic changes the food consumption patterns" has been among 21 selected achievements in the field of interdisciplinary research by the Slovenian Research Agency.

3. Boško Koloski in Bojan Evkoski: Prize for winning the GreenHack Hecaton
4. Adem Kikaj in Marko Bohanec: Award for the best student contribution at the ICDSST 2021 conference

INTERNATIONAL PROJECTS

1. ParlaMint - Towards Comparable Parliamentary Discourse
   Prof. Tomaž Erjavec
   Clarin Eric
2. INEA/CEF - MaCoCu; Massive Collection and Curation of Monolingual and Bilingual Data: Focus on Under-Resourced Languages
   Dr. Nikola Ljubešić
   Innovation And Networks Executive Agency (inea)
3. ParlaMint II - Towards Comparable Parliamentary Corpora
   Prof. Tomaž Erjavec
   Clarin Eric
4. COST CA16204; Distant Reading for European Literary History
   Prof. Tomaž Erjavec
   Cost Association Aisbl
5. COST CA18237; European Soil-Biology Data Warehouse for Soil Protection
   Prof. Marko Debeljak
   Cost Association Aisbl
6. CLARIN Resource Families (Secondment Agreement for Prof. Dr. Darja Fišer)
   Prof. Darja Fišer
   Clarin Eric
7. CLARIN Resource Families (Secondment Agreement for Dr. Jakob Lenardič)
   Dr. Jakob Lenardič
   Clarin Eric
8. E-COST-GRANT-CA18237-66EEBF07; Network Analysis of Pristine Soil Biota
   Prof. Marko Debeljak
   Cost Association Aisbl
9. H2020 - TRUE; Transition Paths to Sustainable Legume based Systems in Europe
   Prof. Marko Debeljak
   European Commission
10. H2020 - TomRes; A Novel and Integrated Approach to increase Multiple and Combined Stress Tolerance in Plants Using Tomato as a Model
    Prof. Marko Debeljak
    European Commission
11. H2020 - NARSIS; New Approach to Reactor Safety Improvements
    Prof. Marko Bohanec
    European Commission
12. H2020 - SAAM; Supporting Active Ageing through Multimodal Coaching
    Asst. Prof. Bernard Ženko
    European Commission
13. H2020 - AI4EU; A European AI On Demand Platform and Ecosystem
    Prof. Sašo Džeroski
    European Commission
14. H2020 - RESILOC; Resilient Europe and Societies by Innovating Local Communities
    Dr. Aljaž Osojnik
    European Commission
15. H2020 - FNS-Cloud; Food Nutrition Security Cloud
    Prof. Nada Lavrač
    European Commission
16. H2020 - HECAT; Disruptive Technologies Supporting Labour Market Decision Making
    Prof. Biljana Mileva Boshkoska
    European Commission
17. H2020 - TAILOR; Foundations of Trustworthy AI - Integrating Reasoning, Learning and Optimization
    Prof. Sašo Džeroski
    European Commission
18. H2020 - COCOREADO; Connecting COnsumers and producers to REbalance farmers
    Prof. Marko Debeljak
    European Commission
19. H2020 - RADIANT; ReAlising DynamIc vAlue chaiNs for underuTilised crops
    Prof. Marko Debeljak
    European Commission
20. H2020 - EMBEDDIA; Cross-Lingual Embeddings for Less-Represented Languages in European News Media
    Asst. Prof. Senja Pollak
    European Commission
21. H2020 - IMSyPP; Innovative Monitoring Systems and Prevention Policies of Online Hate Speech

Asst. Prof. Petra Kralj Novak
European Commission

RESEARCH PROGRAMME

1. Knowledge Technologies
   Prof. Sašo Džeroski

R&D GRANTS AND CONTRACTS

1. TermFrame: Terminology and Knowledge Frames across Languages
   Asst. Prof. Senja Pollak
2. The linguistic landscape of hate speech on social media
   Prof. Tomaž Erjavec
3. Quantitative and qualitative analysis of the unregulated corporate financial reporting
   Asst. Prof. Senja Pollak
4. Tradition and Innovation: Traditional Paremiological Units in Dialogue with Contemporary Use
   Prof. Tomaž Erjavec
5. CRISPR/CAS9-mediated targeted mutagenesis for resistance of grapevine and potatoagainst phytoplasmas
   Prof. Nada Lavrač
6. Determining the origin of lever metastases from liquid biopsy
   Prof. Sašo Džeroski
7. Application of single cell sequencing and machine learning in mammary gland biology
   Prof. Sašo Džeroski
8. Hate speech in contemporary conceptualizations of nationalism, racism, gender and migration
   Asst. Prof. Senja Pollak
9. Formant Combinatorics in Slovenian
   Asst. Prof. Senja Pollak
10. Semantic Data Mining for Linked Open Data Science
    Prof. Nada Lavrač
11. Improving Reproducibility of Experiments and Reusability of Research Outputs in Complex Data Analysis
    Asst. Prof. Panče Panov
12. Neuropsychological dysfunctions caused by low level exposure to selected environmental pollutants in susceptible population – NEURODYS
    Prof. Sašo Džeroski
13. Restoration of moldy canvas paintings: improvement or deterioration?
    Prof. Sašo Džeroski
14. Automating the Synthesis and Analysis of Scientific Models
    Prof. Sašo Džeroski
15. Predictive clustering on data streams
    Prof. Sašo Džeroski
16. Computer-assisted multilingual news discourse analysis with contextual embeddings
    Asst. Prof. Senja Pollak
17. Innovative isotopic techniques for identification of sources and biogeochemical cycling of mercury in contaminated sites – IsoCont
    Prof. Sašo Džeroski
18. Human Rights and Regulation of Trustworthy Artificial Inteligence
    Prof. Ljupčo Todorovski
19. Clinical course and outcome of Covid-19
    Prof. Sašo Džeroski
20. RI-SI ELIXIR: Development of research Infrastructure for the international competitiveness of Slovenian RRI space - RI-SI
    Prof. Sašo Džeroski
    Ministry of Education, Science and Sport
21. Development of Slovene in the digital environment
    Prof. Tomaž Erjavec
    Ministry of Culture
22. RI-SI-CLARIN: Development of research Infrastructure for the international competitiveness of Slovenian RRI space - RI-SI CLARIN
    Prof. Tomaž Erjavec
    Ministry of Education, Science and Sport
23. Human Rights and Regulation of Trustworthy Artificial Inteligence
    Prof. Ljupčo Todorovski
    Ministry of Public Administration
24. Clinical course and outcome of Covid-19
    Prof. Sašo Džeroski
    Ministry of Health
25. Human Rights and Regulation of Trustworthy Artificial Inteligence

Prof. Ljupčo Todorovski
Ministry of Education, Science and Sport
26. Human Rights and Regulation of Trustworthy Artificial Inteligence
Prof. Ljupčo Todorovski
Ministry of Justice

NEW CONTRACTS

1. Multicriteria decision modeling for transparent tunnel design
   Asst. Prof. Bernard Ženko
   Elea Ic d. o. o.
2. Machine learning for Predicting Spacecraft Subsystem Power Consumption
   Prof. Sašo Džeroski
   Bias Variance Labs d. o. o.
3. AI4EO prototyping enviroment for Earth Observation
   Prof. Sašo Džeroski
   Bias Variance Labs d. o. o.

STAFF

Researchers
1. Prof. Marko Bohanec
2. Dr. Michelangelo Ceci
3. Prof. Bojan Cestnik*
4. Prof. Marko Debeljak
5. **Prof. Sašo Džeroski, Head**
6. Prof. Tomaž Erjavec
7. Prof. Darja Fišer*
8. Asst. Prof. Aneta Ivanovska
9. Dr. Dragi Kocev
10. Prof. Nada Lavrač
11. Prof. Zoran Levnajić*
12. Dr. Nikola Ljubešić
13. Prof. Igor Mozetič
14. Asst. Prof. Panče Panov
15. Dr. Vid Podpečan
16. Asst. Prof. Senja Pollak
17. Dr. Matthew Richard John Purver
18. Prof. Ljupčo Todorovski*
19. Prof. Tanja Urbančič*
20. Dr. Ana Zwitter Vitez*
21. Asst. Prof. Bernard Ženko
22. Asst. Prof. Martin Žnidaršič
23. **Postdoctoral associates**
24. Dr. Martin Breskvar
25. *Dr. Jan Kralj*, left 01.12.21*
26. Asst. Prof. Petra Kralj Novak
27. Dr. Janez Kranjc
28. Dr. Vladimir Kuzmanovski
29. Dr. Jakob Lenardič*
30. Prof. Biljana Mileva Boshkoska
31. Dr. Aljaž Osojnik
32. Dr. Matej Petković
33. Dr. Nikola Simidjievski
34. *Dr. Tomaž Stepišnik, left 17.05.21*
35. Dr. Jovan Tanevski
36. Dr. Anita Valmarska*
37. **Postgraduates**
38. Jure Brence, B. Sc.
39. Tanja Dergan, B. Sc.
40. Enja Kokalj, B. Sc.
41. Ana Kostovska, B. Sc.
42. Taja Kuzman, B. Sc.
43. Matej Martinc, B. Sc.
44. Martin Marzidovšek, M. Sc.
45. Katja Meden, B. Sc.
46. Nina Omejc, M. Sc.
47. Andraž Pelicon, B. Sc.
48. Andraž Repar*, B. Sc.
49. Blaž Škrlj, B. Sc.
50. Tadej Škvorc, B. Sc.
51. **Technical officers**
52. Tina Anžič, B. Sc.
53. Nika Eržen, B. Sc.
54. Peter Rupnik, B. Sc.
55. **Technical and administrative staff**
56. Milica Bauer, B. Sc.

Note:
* part-time JSI member

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Original Article

1. Bojan Evkoski, Nikola Ljubešić, Andraž Pelicon, Igor Mozetič, Petra Kralj Novak, "Evolution of topics and hate speech in retweet network communities", *Applied network science*, 2021, **6**, 96.
2. Matej Petković, Blaž Škrlj, Dragi Kocev, Nikola Simidjievski, "Fuzzy Jaccard index: a robust comparison of ordered lists", *Applied soft computing*, 2021, **113**, a, 107849.
3. Anita Peti-Stantić, Maja Anđel, Vedrana Gnjidić, Gordana Keresteš, Nikola Ljubešić, Irina Masnikosa, Mirjana Tonković, Jelena Tušek, Jana Willer-Gold, Mateusz Milan Stanojević, "The Croatian psycholinguistic database: estimates for 6000 nouns, verbs, adjectives and adverbs", *Behavior research methods*, 2021, **53**, 1799-1816.
4. Tome Eftimov, Bibek Paudel, Gorjan Popovski, Dragi Kocev, "A framework for evaluating personalized ranking systems by fusing different evaluation measures", *Big data research*, 2021, **25**, 100211.
5. Blaž Škrlj, Nika Eržen, Nada Lavrač, Tanja Kunej, Janez Konc, "CaNDis: a web server for investigation of causal relationships between diseases, drugs, and drug targets", *Bioinformatics*, 2021, **36**, 6, 885-887.
6. Sebastian Mežnar, Nada Lavrač, Blaž Škrlj, "Transfer learning for node regression applied to spreading prediction", *Complex systems*, 2021, **30**, 4, 457-481.
7. Matej Martinc, Senja Pollak, Marko Robnik Šikonja, "Supervised and unsupervised neural approaches to text readability", *Computational linguistics*, 2021, **47**, 1, 141-179.
8. Blaž Škrlj, Matej Martinc, Jan Kralj, Nada Lavrač, Senja Pollak, "tax2vec: constructing interpretable features from taxonomies for short text classification", *Computer speech & language*, 2021, **65**, 101104.
9. Fasih Haider, Senja Pollak, Pierre Albert, Saturnino Luz, "Emotion recognition in low-resource settings: an evaluation of automatic feature selection methods", *Computer speech & language*, 2021, **65**, 101119.
10. Tomaž Stepišnik, Blaž Škrlj, Jörg Wicker, Dragi Kocev, "A comprehensive comparison of molecular feature representations for use in predictive modeling", *Computers in Biology and Medicine*, 2021, **130**, 104197.
11. Tim Smole *et al.* (19 authors), "A machine learning-based risk stratification model for ventricular tachycardia and heart failure in hypertrophic cardiomyopathy", *Computers in Biology and Medicine*, 2021, **135**, 104648.
12. Jean-Philippe Deguine, Marie-Hélène Robin, David Camilo Corrales, Marie-Anne Vedy-Zecchini, Anna Doizy, Frédéric Chiroleu, Gauthier

Quesnel, Isaure Païtard, Marko Bohanec, Jean-Noël Aubertot, "Qualitative modeling of fruit fly injuries on chayote in Réunion: development and transfer to users", *Crop protection*, 2021, **139**, 105367.

13. Rok Piltaver, Mitja Luštrek, Sašo Džeroski, Martin Gjoreski, Matjaž Gams, "Learning comprehensible and accurate hybrid trees", *Expert systems with applications*, 2021, **164**, 113980.

14. Marko Bohanec *et al.* (11 authors), "HeartMan DSS: a decision support system for self-management of congestive heart failure", *Expert systems with applications*, 2021, **186**, 115688.

15. Matej Martinc, Fasih Haider, Senja Pollak, Saturnino Luz, "Temporal integration of text transcripts and acoustic features for Alzheimer's diagnosis based on spontaneous speech", *Frontiers in aging neuroscience*, 2021, **13**, 652647.

16. Octave Lacroix, Jean-Noël Aubertot, Marko Bohanec, Stéphane Cordeau, David Camilo Corrales, Marie-Hélène Robin, "IPSIM-Cirsium, a qualitative expert-based model to predict infestations of *Cirsium arvense*", *Frontiers in agronomy*, 2021, **3**, 655383.

17. Shamila Nasreen, Morteza Rohanian, Julian Hough, Matthew Purver, "Alzheimer's dementia recognition from spontaneous speech using disfluency and interactional features", *Frontiers in computer science*, 2021, **3**, 640669.

18. Taru Sandén, Anna Wawra, Helene Berthold, Julia Miloczki, Agnes Schweinzer, Brigitte Gschmeidler, Heide Spiegel, Marko Debeljak, Aneta Trajanov, "TeaTime4Schools: using data mining techniques to model litter decomposition in austrian urban school soils", *Frontiers in ecology and evolution*, 2021, **9**, 703794.

19. Blaž Škrlj, Enja Kokalj, Nada Lavrač, "PubMed-scale chemical concept embeddings reconstruct physical protein interaction networks", *Frontiers in research metrics and analytics*, 2021, **6**, 644614.

20. Pietro Iannetta *et al.* (18 authors), "A multifunctional solution for wicked problems: value-chain wide facilitation of legumes cultivated at bioregional scales is necessary to address the climate-biodiversity-nutrition nexus", *Frontiers in sustainable food systems*, 2021, **5**, 692137.

21. Martin Breskvar, Sašo Džeroski, "Multi-target regression rules with random output selections", *IEEE access*, 2021, **9**, 10509-10522.

22. Miljenko Hajnić, Biljana Mileva Boshkoska, "A disruptive decision support platform for reengineering the strategic transfer of employees", *IEEE access*, 2021, **9**, 29921-29928.

23. Marius Schwabenland *et al.* (26 authors), "Deep spatial profiling of human COVID-19 brains reveals neuroinflammation with distinct microanatomical microglia-T-cell interactions", *Immunity*, 2021, **54**, 7, 1593-1610.

24. Swati Swati, Dunja Mladenić, Tomaž Erjavec, "EveOut: an event-centric news dataset to analyze an outlet's event selection patterns", *Informatica: an international journal of computing and informatics*, 2021, **45**, 7, 25-30.

25. Roberto Corizzo, Michelangelo Ceci, Hadi Fanaee-T, João Gama, "Multi-aspect renewable energy forecasting", *Information sciences*, 2021, **546**, 701-722.

26. Matej Petković, Dragi Kocev, Blaž Škrlj, Sašo Džeroski, "Ensemble- and distance-based feature ranking for unsupervised learning", *International journal of intelligent systems*, 2021, **36**, 7, 3068-3096.

27. Marina Dermastia *et al.* (16 authors), "Differential response of grapevine to Infection with '*Candidatus Phytoplasma solani*' in early and late growing season through complex regulation of mRNA and small RNA transcriptomes", *International journal of molecular sciences*, 2021, **22**, 7, 3531.

28. Mitja Luštrek *et al.* (21 authors), "A personal health system for self-management of congestive heart failure (HeartMan): development, technical evaluation, and proof-of-concept randomized controlled trial", *JMIR medical informatics*, 2021, **9**, 3, e24501.

29. Janez Konc, Samo Lešnik, Blaž Škrlj, Dušanka Janežič, "ProBiS-Dock database: a web server and interactive web repository of small ligand-protein binding sites for drug design", *Journal of chemical information and modeling*, 2021, **61**, 8, 4097-4107.

30. Matej Radinja, Mateja Škerjanec, Mojca Šraj, Sašo Džeroski, Ljupčo Todorovski, Nataša Atanasova, "Automated modelling of urban runoff based on domain knowledge and equation discovery", *Journal of Hydrology*, 2021, **603**, 127077.

31. Matthew Purver, Mehrnoosh Sadrzadeh, Ruth M. Kempson, Gijs Wijnholds, Julian Hough, "Incremental composition in distributional semantics", *Journal of logic, language and information*, 2021, **30**, 379-407.

32. Jure Brence, Ljupčo Todorovski, Sašo Džeroski, "Probabilistic grammars for equation discovery", *Knowledge-based systems*, 2021, **224**, 107077.

33. Tomaž Stepišnik, Dragi Kocev, "Oblique predictive clustering trees", *Knowledge-based systems*, 2021, **227**, 107228.

34. Pavle Boškoski, Matija Perne, Martina Rameša, Biljana Mileva Boshkoska, "Variational Bayes survival analysis for unemployment modelling", *Knowledge-based systems*, 2021, **229**, 107335.

35. Blaž Škrlj, Matej Martinc, Nada Lavrač, Senja Pollak, "autoBOT: evolving neuro-symbolic representations for explainable low resource text classifcation", *Machine learning*, 2021, **110**, 4, 989–1028.

36. Darja Fišer, Nikola Ljubešić, Damjan Popič, "From fringe to infrastructure: a researcher's journey through South Slavic language attitudes on social media", *Modern languages open*, 2021, **1**, 24.

37. Christoph Schöch, Roxana Patraş, Tomaž Erjavec, Diana Santos, "Creating the European Literary Text Collection (ELTeC)", *Modern languages open*, 2021, **1**, 25.

38. Attila Gabor *et al.* (10 authors), "Cell-to-cell and type-to-type heterogeneity of signaling networks: insights from the crowd", *Molecular systems biology*, 2021, **17**, 10, e10402.

39. Marko Jukič, Blaž Škrlj, Gašper Tomšič, Sebastian Pleško, Črtomir Podlipnik, Urban Bren, "Prioritisation of compounds for 3CL[pro] inhibitor development on SARS-CoV-2 variants", *Molecules*, 2021, **26**, 10, 3003.

40. Matej Martinc, Blaž Škrlj, Senja Pollak, "TNT-KID: transformer-based neural tagger for keyword identification", *Natural language engineering*, 2021, **28**, 4, 409-448.

41. Tom Vermeyen, Jure Brence, Robin Van Echelpoel, Roy Aerts, Guillaume Acke, Patrick Bultinck, Wouter Herrebout, "Exploring machine learning methods for absolute configuration determination with vibrational circular dichroism", *PCCP. Physical chemistry chemical physics*, 2021, **23**, 354, 19781-19789.

42. Tomaž Stepišnik, Dragi Kocev, "Semi-supervised oblique predictive clustering trees", *PeerJ computer science*, 2021, e506.

43. Andraž Pelicon, Ravi Shekhar, Blaž Škrlj, Matthew Purver, Senja Pollak, "Investigating cross-lingual training for offensive language detection", *PeerJ computer science*, 2021, e559.

44. Blaž Škrlj *et al.* (11 authors), "New cross-talks between pathways involved in grapevine infection with '*Candidatus Phytoplasma solani*' revealed by temporal network modelling", *Plants*, 2021, **10**, 4, 646.

45. Bojan Evkoski, Igor Mozetič, Nikola Ljubešić, Petra Kralj Novak, "Community evolution in retweet networks", *PloS one*, 2021, **16**, 9, e0256175.

46. Darja Fišer, Kristina Pahor de Maiti, ""Prvič, sem političarka in ne politik, drugič pa — ": korpusni pristop k raziskovanju parlamentarnega diskurza", *Prispevki za novejšo zgodovino*, 2021, **61**, 1, 144-179.

47. Mojca Šorn, Katja Meden, "Portal Zgodovina Slovenije - SIstory in avtorske pravice", *Prispevki za novejšo zgodovino*, 2021, **61**, 2, 193-228.

48. Tanja Mesti, Vid Čeplak Mencin, Biljana Mileva Boshkoska, Janja Ocvirk, "Adverse events during immunotherapy in Slovenian patients with metastatic melanoma reveal a positive correlation with better treatment outcomes", *Radiology and oncology*, 2021, **55**, 3, 354-361.

49. Els Clays *et al.* (21 authors), "Proof-of-concept trial results of the HeartMan mobile personal health system for self-management in congestive heart failure", *Scientific reports*, 2021, **11**, 5663.

50. Matteo Cinelli, Andraž Pelicon, Igor Mozetič, Walter Quattrociocchi, Petra Kralj Novak, Fabiana Zollo, "Dynamics of online hate and misinformation", *Scientific reports*, 2021, **11**, 22083.

51. Zdravko Kunić, Bernard Ženko, Biljana Mileva Boshkoska, "FOCUSED-short-term wind speed forecast correction algorithm based on successive nwp forecasts for use in traffic control decision support systems", *Sensors*, 2021, **21**, 10, 3405.

52. Janja Polajnar, Darja Fišer, "Samoreference v akademski slovenščini: kvantitativno-kvalitativna korpusna analiza rabe prvoosebnih edninskih in množinskih oblik", *Slavistična revija: časopis za jezikoslovje in literarne vede*, 2021, **69**, 4, 414-430.

53. Marko Robnik Šikonja, Kristjan Reba, Igor Mozetič, "Cross-lingual transfer of sentiment classifiers", *Slovenščina 2.0: empirične, aplikativne in interdisciplinarne raziskave*, 2021, **9**, 1, 1-25.

54. Matej Ulčar, Anka Supej, Marko Robnik Šikonja, Senja Pollak, "Slovene and Croatian word embeddings in terms of gender occupational analogies", *Slovenščina 2.0: empirične, aplikativne in interdisciplinarne raziskave*, 2021, **9**, 1, 26-59.

55. Jakob Lenardič, Darja Fišer, "Hedging modal adverbs in Slovenian academic discourse", *Slovenščina 2.0: empirične, aplikativne in interdisciplinarne raziskave*, 2021, **9**, 1, 145-180.

56. Katja Meden, Ana Cvek, "Nadgradnja zgodovinarskega indeksa citiranosti", *Slovenščina 2.0: empirične, aplikativne in interdisciplinarne raziskave*, 2021, **9**, 1, 216-235.

57. Matej Petković, Gorjan Popovski, Barbara Koroušić-Seljak, Dragi Kocev, Tome Eftimov, "DietHub: dietary habits analysis through understanding the content of recipes", *Trends in food science & technology*, 2021, **107**, 183-194.

58. Ana Zwitter Vitez, "L'expression de l'opinion: analyse textuelle, syntaxique et lexicale de réactions àun événement politique", *Vestnik za tuje jezike*, 2021, **13**, 1, 91-108.

59. Matej Radinja, Mateja Škerjanec, Sašo Džeroski, Ljupčo Todorovski, Nataša Atanasova, "Design and simulation of stormwater control measures using automated modeling", *Water*, 2021, **13**, 16, 2268.

60. Michelangelo Ceci, Pasqua Fabiana Lanotte, "Closed sequential pattern mining for sitemap generation", *World wide web*, 2021, **24**, 1, 175-203.

REVIEW ARTICLE

1. Nikolaja Janež, Blaž Škrlj, Meta Sterniša, Anja Klančnik, Jerica Sabotič, "The role of the *Listeria* monocytogenes surfactome in biofilm formation", *Microbial biotechnology*, 2021, **14**, 4, 1269-1281.

PUBLISHED CONFERENCE CONTRIBUTION

1. Martin Žnidaršič, Aljaž Osojnik, Peter Rupnik, Bernard Ženko, "Improving effectiveness of a coaching system through preference learning", In: *PETRA 2021, 14th ACM International Conference on PErvasive Technologies related to Assistive Environments, June 29-July 1, 2021*, ACM, 2021, 459-465.

2. Bojan Cestnik, Andreja Abina, Rebeka Kovačič Lukman, Aleksander Zidanšek, "Expert system for systematic monitoring of sustainability-related competences in higher education", In: *16th Conference on Sustainable Development of Energy, Water and Environment Systems (SDEWES), 10-15 October 2021, Dubrovnik, Croatia*, Faculty of Mechanical Engineering and Naval Architecture, 2021.

3. Timen Stepišnik Perdih, Nada Lavrač, Blaž Škrlj, "Semantic reasoning from model-agnostic explanations", In: *2021 IEEE 19th World Symposium on Applied Machine Intelligence and Informatics (SAMI), 21-23 January 2021*, Proceedings, IEEE, 105-110.

4. Yujian Gan, Xinyun Chen, Qiuping Huang, Matthew Purver, John R. Woodward, Jinxia Xie, Huang Pengsheng, "Towards robustness of Text-to-SQL models against synonym substitution", In: *ACL-IJCNLP 2021, 59th Annual Meeting of the Association for Computational Linguistics and 11th International Joint Conference on Natural Language Processing, August 1-6, 2021*, Proceedings, Association for Computational Linguistics, 2021, Vol. 1, 2505-2515.

5. Vladimir Kuzmanovski, Jaakko Hollmén, "Composite surrogate for likelihood-free Bayesian optimisation in high-dimensional settings of activity-based transportation models", In: *IDA 2021, 19th International Symposium on Intelligent Data Analysis, Porto, Portugal, April 26-28, 2021*, Advances in Iintelligent Data Analysis XIX, (Lecture Notes in Computer Science **12695**), Springer, 2021, 171-183.

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THESES AND MENTORING

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2. Jaka Čibej, *Korpusna analiza in prepoznavanje regionalnih jezikovnih različic v spletni slovenščini:* doctoral dissertation, Ljubljana, 2021 (mentor Darja Fišer; co-mentor Vojko Gorjanc).

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DEPARTMENT OF INTELLIGENT SYSTEMS

E-9

The Department of Intelligent Systems develops new methods and techniques for intelligent computer systems, with applications in the areas of the information society, computer science and informatics, and network communication systems. The main research areas are ambient intelligence, agent and multi-agent systems, computational intelligence, language and speech technologies, electronic and mobile health, and smart cities. The department closely collaborates with the Faculty of Computer and Information Science of the University of Ljubljana in the joint research programme "Artificial Intelligence and Intelligent Systems". The department also collaborates with industry and contributes to the inclusion of intelligent systems in products and services.

Head:
Prof. Matjaž Gams

Intelligent systems simulate intelligence so that a typical user perceives them as truly intelligent. In reality, these systems use complex mechanisms and implement them on digital platforms to imitate human behaviour by exploiting raw, exponentially growing computer power. This field is somewhat broader than artificial intelligence, but both are rapidly growing worldwide and are enabling the development of the information society.

Ambient intelligence is a research field aiming to introduce technology into our everyday environment in a friendly way that is undemanding for the user. The main area where the department applies methods of ambient intelligence is health. We finished the H2020 project **WellCo**, within which we created a virtual coach to advise elder users on wellbeing and health. For this coach we developed methods for monitoring nutrition with sensors and questionnaires, recognizing users' emotions from their voice, and identifying trends and anomalies in health behaviour. We also finished the H2020 project **Insension** intended to help people with severe intellectual disability to use digital services. We developed methods for the interpretation of their inner state using the video from cameras and other sensors. In the newly started H2020 project **WideHealth** we engage in training and networking activities regarding pervasive health and related topics. In the Flemish-Slovenian project **STRAW**, whose objectives are stress recognition from sensor data and analysis of stressors in the workplace we concluded data collection with a sensing wristband and a mobile application, and started the data analysis.

We came second in the \$500k XPrize Pandemic Response Challenge, a competition whose goal was to develop methods that can predict Covid-19 infections and recommend non-pharmacological interventions with optimal trade-offs between effectiveness and socio-economic cost.

In the AAL project **CoachMyLife** we help seniors with memory impairment perform everyday tasks. To this end, we developed methods for assisting with the kitchen activities using computer vision and a sensing wristband. In the H2020 project **COVIRNA** we started to develop a diagnostic test for cardiovascular patients with Covid-19. Related to Covid-19 we came second in the **XPrize Pandemic Response Challenge**, winning 250,000 USD. The goal of the competition was to develop methods that predict infections and recommend a non-pharmacological intervention with optimal trade-offs between effectiveness and socio-economic cost. We pursue **doctoral research** on the contact-free sensing of physiological signals and states, and on selecting questions for nutrition questionnaires in a way that obtains most information with fewest questions, and on stress modelling.

In the field of **agent and multi-agent systems**, the key research areas are the development of intelligent autonomous systems for managing smart cities, and intelligent healthcare-support systems. These require the development of new algorithms, methods and approaches, introducing artificial intelligence into computer systems. In the Interreg Italy-Slovenia project **Insieme**, we are developing a platform for electronic and mobile health (EMH), which offers Slovenian and Italian users a range of online services, including the possibility of talking online with specialists in the field of EMH. We also developed several new and innovative devices and solutions to support elderly and chronic patients at home where, among other things, we

Figure 1: We have described and analyzed a suite of bi-objective optimization benchmark problems. The figure shows two landscape properties for its function F10, a combination of the sphere function and the Gallagher function with 101 peaks.

already developed a smartwatch for the elderly, but we are now transferring it to mobile phones. In addition to the improvements to the system for an autonomic reaction after a fall, we also introduced a system for predicting falls, which uses the bracelet to determine the stability of walking and, in the event of deterioration, warn of the risk of falling. For the H2020 **URBANITE** smart cities project, we are developing a system that simulates traffic, and validates

Figure 2: We help the Comland company develop fieldwork scheduling software that has to consider a variety of criteria and constraints.

We completed the bilateral Slovenian-German project Multiobjective Optimization for Artificial Intelligence Systems in Industry, investigating the potentials of a multiobjective optimization methodology in the design of cyclone dust separators and elevator group control systems.
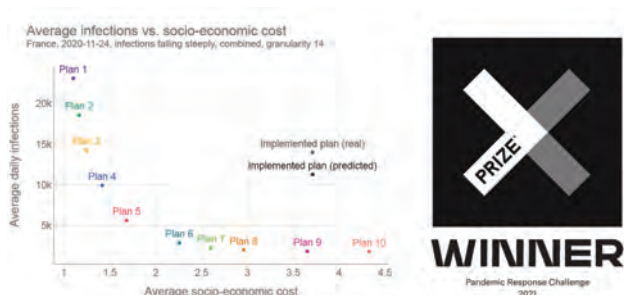
Figure 3: Predicting socio-economic cost and efficiency of an intervention plan against Covid-19. Besides evaluating a given intervention plan, we also suggest numerous alternative plans that are more effective at the same cost. With this work, we have won the »$500K Pandemic Response Challenge«.
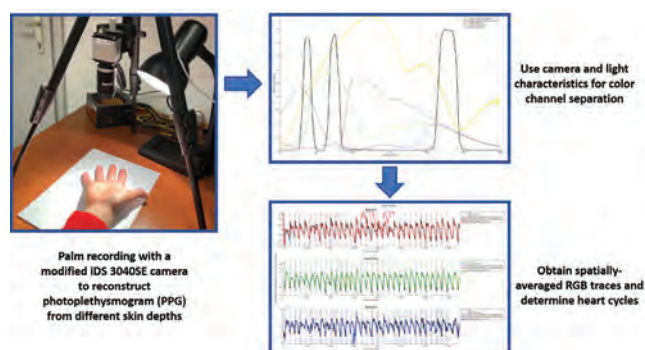
Figure 4: Contact-free reconstruction of photoplethysmograms from various skin layers at different depths using a modified RGB camera and leveraging various light wavelengths

and identifies the best mobility policies and measures. The project includes four European cities: Amsterdam, Helsinki, Bilbao and Messina. As part of the European ERA PerMed **BATMAN** project, where the aim is the Acne Inversa disease research, we developed and deployed a system for data collection, visualization and analysis. The system is used by the physicians from the European partners and their patients. The goal is to create a sufficiently large database for processing, using AI methods. In the H2020 **PlatformUptake. eu** project, we developed a method for clustering open platforms in the field of active and healthy ageing. We successfully concluded the **ROBKONCEL** project by delivering an intelligent system for comprehensive quality control in production, using a reconfigurable robotic control cell and an intelligent process control module, to the project partners Gorenje and Unior.

Computational intelligence is a study of stochastic search, optimization and learning methods, inspired by biological and physical systems. The research in this area at the Department of Intelligent Systems focuses on evolutionary computation and optimization. We study evolutionary algorithms for multiobjective optimization, their acceleration through parallel computing and surrogate models, constraint handling in multiobjective optimization, visualization of optimization results, methodology of algorithm benchmarking, and their applicability in science and engineering. In 2021, we started researching the **characterization of constrained multiobjective optimization problems**. After extending the landscape analysis to multiobjective optimization, we studied the properties of the test problem suites and evaluated their quality for the purpose of optimization algorithm benchmarking. We also continued our research on **optimization algorithm benchmarking** by investigating the properties of bi-objective optimization benchmark problems included in the open-source COCO (Comparing Continuous Optimizers) platform. The results 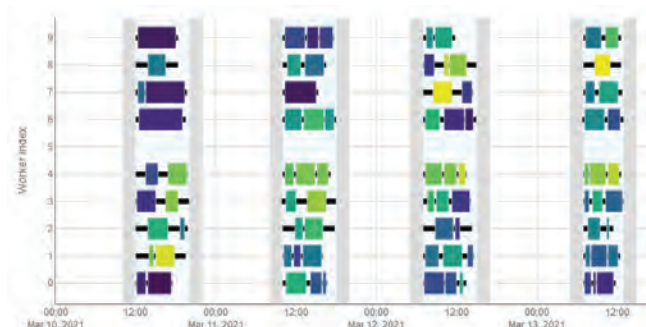of this analysis include various problem landscape visualizations and are presented at a dedicated website (https://numbbo.github.io/bbob-biobj/). In the Slovenian-German project **Multiobjective Optimization for Artificial Intelligence Systems in Industry** carried out together with the Cologne University of Applied Sciences (TH Köln) and finished in 2021, we investigated the potentials of a multiobjective optimization methodology in manufacturing and transportation. Of our particular interest was the optimization of cyclone dust separators and elevator group control systems. The project resulted in joint publications and organization of specialized events at major international conferences on evolutionary computation. Finally, we started working on the project **Intelligent and Environmentally Friendly Scheduling of Field Work (MF-Scheduler)** for the Comland company, which entails solving a demanding routing and scheduling problem. We assisted the company in defining the problem as a mixed-integer linear program. We also provide expertise in managing the combinatorial complexity of problems and are developing a module for the meta-optimization of optimization algorithm parameters.

In the field of **speech and language technologies**, we work on speech synthesis, semantic analysis of text and question answering. Together with the companies Alpineon and Amebis we developed a new, high-quality speech synthesizer **eBralec** (http://ebralec.si/). The software package has more than a thousand subscribers and is an indispensable tool for blind and visually impaired users (it is the "official" speech synthesizer of the Slovenian Association for the Blind and Visually Impaired) and people with reading impairments (the Bravo association). For these users, eBralec is free of charge and can be ordered at the Library for the Blind and Visually Impaired (http://www.kss-ess.si/ebralec-sintetizator-govora-slovenskega-jezika/). eBralec is also an integral part of the DarsTraffic+ application, which provides traffic information, while its server version has been used by the National and University Library since 2017. It has been reading news on the renewed Delo (national daily newspaper) website. We completed successfully the **AudiBook** project: "Education accessibility through a digital audio library for the blind and visually impaired".

The **24th International Multiconference Information Society – IS 2021** (is.ijs.si) took place at the Jožef Stefan Institute on 4–8 October 2021. It consisted of 11 independent conferences with 150 presentations. Four conference awards were presented: The award for lifelong outstanding contributions was presented in memory of Donald Michie and Alan Turing. The Michie-Turing Award was presented to Prof. Dr Jernej Kozak for his lifelong outstanding contribution to the development and promotion of the information society in our country. In addition, the yearly recognition for current achievements was awarded to the team from the Department of Intelligent Systems, Jožef Stefan Institute, for winning the second place at the XPrize Pandemic Response Challenge for proposing best counter-measures against the Covid-19 pandemic. The information lemon went to the claim that the mobile application for tracking Covid-19 contacts will harm information privacy. The information strawberry for best information service last year went to Covid-19 Sledilnik, a program regularly reporting all the data related to Covid-19 in Slovenia.
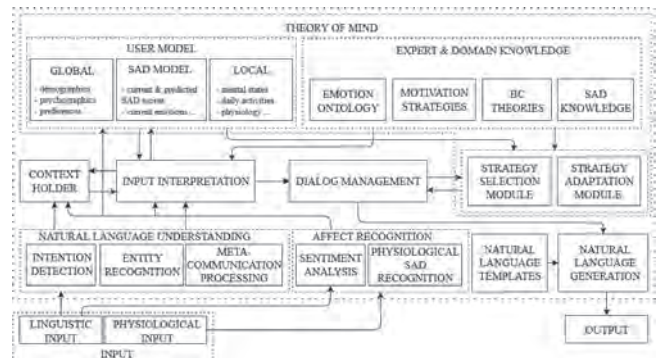
Figure 5: Cognitive architecture of an assistant for changing mental health behavior

Figure 6: At the 24th International Multiconference Information Society, IS 2021, the Donald Michie and Alan Turing award was presented to Prof. Dr Jernej Kozak for his lifelong outstanding contributions.

Figure 7: Yearly recognition for current achievements at the multiconference IS 2021 was awarded to the team from the Department of Intelligent Systems for the second place at the XPrize Pandemic Response Challenge for proposing best counter-measures against the COVID-19 pandemic.

Some outstanding publications in the past year

1. Badimon, L., Luštrek, M., et al., On behalf of EU-CardioRNA COST Action CA17129. Cardiovascular RNA markers and artificial intelligence may improve COVID-19 outcome: a position paper from the EU-CardioRNA COST Action CA17129. Cardiovascular Research, 2021, 117 (8), 1823–1840

2. Bohanec, M., Vodopija, A., Luštrek, M., et al. HeartMan DSS: A decision support system for self-management of congestive heart failure. Expert Systems with Applications, 2021, 186, 115688-1–115688-13

3. Hansen, N., Auger, A., Ros, R., Mersmann, O., Tušar, T., Brockhoff, D. COCO: A platform for comparing continuous optimizers in a black-box setting. Optimization Methods & Software, 2021, 36 (1), 114–144

4. Koblar, V., Filipič, B. Evolutionary design of a system for online surface roughness measurements. Mathematics, 2021, 9 (16), 1904

5. Piltaver, R., Luštrek, M., Džeroski, S., Gjoreski, M., Gams, M. Learning comprehensible and accurate hybrid trees. Expert Systems with Applications, 164, 113980-1–113980-11

Awards and appointments

1. Team JSI vs COVID: Matej Cigale, Carlo De Masi, Erik Dovgan, Matjaž Gams, Anton Gradišek, Vito Janko, Mitja Luštrek, Matej Marinko, Nina Reščič, David Susič, Tea Tušar, Aljoša Vodopija: Second place at the XPrize Pandemic Response Challenge; virtual; XPrize Foundation; methods for predicting COVID-19 infections and recommending countermeasures

2. Nina Reščič, Vito Janko, David Susič, Carlo De Masi, Aljoša Vodopija, Matej Marinko, Tea Tušar, Erik Dovgan, Matej Cigale, Anton Gradišek, Matjaž Gams, Mitja Luštrek: Best paper award at the ETAI 2021 conference; virtual / Skopje, North Macedonia; paper Finding efficient intervention plans against COVID-19

3. Members of the Department of Intelligent Systems, Jožef Stefan Institute: Award for current work in the area of information society; Ljubljana, Slovenia; Programme and organizational committe of the Information Society 2021 multiconference; second place at the XPrize Pandemic Response Challenge

4. Carlo De Masi, Simon Stankoski, Vincent Cergolj, Mitja Luštrek: Best paper award at Slovenian Conference on Artificial Intelligence 2021; Ljubljana, Slovenia; Programme committee of the Slovenian Conference on Artificial Intelligence 2021; paper Intent recognition and drinking detection for assisting kitchen-based activities

5. Matjaž Gams, Urša Klun, Primož Kocuvan, Tine Kolenik : Best paper award of the Insieme project Workshop, Programme and organization committee of the Insieme project Workshop, International multiconference Information Society, IS2021, "Intelligent cognitive assistant technology for (mental) health in the ISE-EMH project"

6. Matjaž Gams, David Susič, Janez Tomšič: Award for best workshop paper of the project Insieme, Ljubljana, Programme and Organizing Committee of the Project Insieme Workshop, International Multiconference Information Society, IS2021, Effectiveness of non-pharmaceutical interventions in handling the COVID-19 pandemic: Review of related studies"

7. Anton Gradišek, Best presentation award at the conference "EcoBalt", Riga, Latvia, 21-23. 10. 2021

Organization of conferences, congresses and meetings

1. 38th Slovenian Workshop on Nature-Inspired Algorithms, AVN, Maribor, 28 May 2021 (virtual)
2. Session on Evolutionary Computation in Practice (ECiP) at the Genetic and Evolutionary Computation Conference, GECCO 2021, Lille, France, 12 July 2021 (virtual)
3. 39th Slovenian Workshop on Nature-Inspired Algorithms, AVN, Ljubljana, 1 October 2021 (virtual)
4. 24th International Multiconference Information Society (IS 2021), Ljubljana, 4–10 October 2021, independent conferences:
   – 50th Anniversary of Teaching Computer Science in Slovenian Secondary Schools
   – Batman Project Workshop
   – Cognitive Science
   – Education in Information Society
   – Insieme Project Workshop
   – International Technology Transfer Conference
   – People and Environment
   – SiKDD Data Mining and Data Warehouses
   – Slovenian Conference on Artificial Intelligence
   – Student Computer Science Research Conference 2021
   – Urbanite Project Workshop

Patent granted

1. Jaka Sodnik, Boštjan Kaluža, Mojca Komavec, Kristina Stojmenova, A driver evaluation procedure and the device for carrying out the procedure, SI25874 (A), Slovenian Intellectual Property Office, 29. 01. 2021.

INTERNATIONAL PROJECTS

1. ERASMUS+; Audio Library for Visually Impaired; Education Accessibility through a Digital Audio Library for the Blind and Visually-Impaired
   Dr. Tomaž Šef
   European Commission
2. ERASMUS+; VALENCE - Advancing Machine Learning in Vocational Education
   Prof. Matjaž Gams
   European Commission
3. COST CA17129: CardioRNA - Catalysing Transcriptomics Research in Cardiovascular Disease
   Dr. Mitja Luštrek
   Cost Association Aisbl
4. H2020 - INSENSION; Personalized Intelligent Platform Enabling Interaction with Digital Services to Individuals with Profound and Multiple Learning Disabilities
   Dr. Mitja Luštrek
   European Commission
5. H2020 - WellCo; Wellbeing and Health Virtual Coach
   Dr. Mitja Luštrek
   European Commission
6. H2020 - PlatformUptake.eu; Assessing the State of Art and Supporting an Evidence-Based Uptake and Evolution of Open Service Platforms in the Active and Healthy Ageing Domain
   Prof. Matjaž Gams
   European Commission
7. H2020 - URBANITE; Supporting the decision-making in URBAN transformation with the use of dIsruptive Technologies
   Prof. Matjaž Gams
   European Commission
8. H2020 - COVIRNA; A Diagnostic Test to improve Surveillance and Care of COVID-19 Patients
   Dr. Mitja Luštrek
   European Commission
9. H2020 - WideHealth; Widening Research on Pervasive and eHealth – WideHealth
   Dr. Mitja Luštrek
   European Commission
10. Development of AI Methods for Monitoring Affective States Using Unobtrusive Sensors
    Prof. Matjaž Gams
    Slovenian Research Agency
11. Multi-Objective Optimization for Artificial Intelligence Systems in Industry
    Prof. Bogdan Filipič
    Slovenian Research Agency

RESEARCH PROGRAMME

1. Artificial Intelligence and Intelligent Systems
   Dr. Mitja Luštrek

R&D GRANTS AND CONTRACTS

1. Precision Medicine Approach to Cell Therapy in Heart Failure
   Asst. Prof. Anton Gradišek
2. Disentangling the sources and context of daily work stress: a comprehensive real-time modelling study using wearbles and technological detections
   Dr. Mitja Luštrek
3. Italian-Slovenian Ecosystem for Electronic and Mobile Health
   Prof. Matjaž Gams
   Regione Autonoma Friuli Venezia Giulia, Direzione
4. Social Innovation for Integrated health CARE of ageing population in ADRION Regions-SI4CARE
   Dr. Mitja Luštrek
   The Emillia-Romagna Region
5. CoachMyLife
   Dr. Mitja Luštrek
   Ministry of Public Administration
6. BATMAN: Biomolecular Analyses for Tailored Medicine in Acne iNversa
   Prof. Matjaž Gams
   Ministry of Education, Science and Sport
7. 24th International Multiconference Information Society 2021, IS 2021, Ljubljana, Slovenia, 4 October 2021 - 8 October 2021
   Prof. Matjaž Gams
8. XPRIZE: JSI vs COVID
   Dr. Mitja Luštrek
   Xprize

NEW CONTRACTS

1. Multicriteria decision modeling for transparent tunnel design
   Asst. Prof. Tea Tušar
   Elea Ic d. o. o.
2. Multiobjective optimization for transparent tunnel design
   Asst. Prof. Tea Tušar
   Xlab d. o. o.
3. Development of reconfigurable robotic cell for final product inspection
   Prof. Matjaž Gams
   Gorenje gospodinjski aparati,d.d.
4. Intelligent and environmentally friendly scheduling of field work - MF-Scheduler
   Prof. Bogdan Filipič
   Comland d. o. o.

STAFF

Researchers
1. Dr. Erik Dovgan
2. Prof. Bogdan Filipič
3. **Prof. Matjaž Gams, Head**
4. Asst. Prof. Anton Gradišek
5. Dr. Mitja Luštrek
6. Dr. Miha Mlakar
7. Dr. Tomaž Šef
8. Asst. Prof. Tea Tušar

Postdoctoral associates
9. Dr. Carlo Maria De Masi
10. Dr. Vito Janko
11. *Dr. Boštjan Kaluža*, left 15.09.21*
12. *Dr. Rok Piltaver*, left 01.11.21*
13. Dr. Aleš Tavčar*

Postgraduates
14. Andrejaana Andova, B. Sc.
15. *Dr. Martin Gjoreski, on leave 01.12.20*
16. Tine Kolenik, B. Sc.
17. *Tomaž Kompara*, B. Sc., left 15.02.21*
18. Dr. Jana Krivec*
19. Gašper Slapničar, B. Sc.

20. David Susič, B. Sc.
21. Aljoša Vodopija, B. Sc.

Technical officers
22. Primož Kocuvan, B. Sc.
23. Žiga Kolar, B. Sc.
24. Anže Marinko, B. Sc.
25. Maj Smerkol, B. Sc.
26. Jakob Valič, B. Sc.
27. Zdenko Vuk, B. Sc.

Technical and administrative staff
28. Jani Bizjak*, B. Sc.
29. *Matej Cigale, B. Sc., left 01.03.21*
30. Vesna Koricki, B. Sc.
31. Mitja Lasič
32. Liljana Lasič
33. Junoš Lukan, M. Sc.
34. Blaž Mahnič, B. Sc.
35. Nina Reščič, B. Sc.
36. Lana Zemljak

Note:
* part-time JSI member

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ORIGINAL ARTICLE

1. Matjaž Gams, Mari Jože Osredkar, "Catholic doctrine and science on demographic issues", *Bogoslovni vestnik: glasilo Teološke fakultete v Ljubljani*, 2021, **81**, 3, 555-567.
2. Gabriel Salierno, Anton Gradišek, Mauricio Maestri, Julia Picabea, Miryan C. Cassanello, Cataldo De Blasio, Maria A. Cardona, Daniel Hojman, Héctor Somacal, "Comparison of the fluidized state stability from radioactive particle tracking results", *ChemEngineering*, 2021, **5**, 4, 65.
3. Jana Krivec, Ivan Bratko, Matej Guid, "Identification and conceptualization of procedural chunks in chess", *Cognitive systems research*, 2021, **69**, 22-40.
4. Tomaž Kompara, Janez Perš, David Susič, Matjaž Gams, "A one-dimensional non-intrusive and privacy-preserving identification system for households", *Electronics*, 2021, **10**, 5, 559.
5. Rok Piltaver, Mitja Luštrek, Sašo Džeroski, Martin Gjoreski, Matjaž Gams, "Learning comprehensible and accurate hybrid trees", *Expert systems with applications*, 2021, **164**, 113980.
6. Marko Bohanec *et al.* (11 authors), "HeartMan DSS: a decision support system for self-management of congestive heart failure", *Expert systems with applications*, 2021, **186**, 115688.
7. Surya Krishnamurthy, K. S. Kapeleshh, Erik Dovgan, Mitja Luštrek, Barbara Gradišek Piletič, Kathiravan Srinivasan, Yu-Chuan (Jack) Li, Anton Gradišek, Shabbir Syed-Abdul, "Machine learning prediction models for chronic kidney disease using national health insurance claim data in Taiwan", *Healthcare*, 2021, **9**, 5, 546.
8. Martin Gjoreski, Bhargavi Mahesh, Tine Kolenik, Jens Uwe-Gabras, Dominik Seuss, Hristijan Gjoreski, Mitja Luštrek, Matjaž Gams, Veljko Pejović, "Cognitive load monitoring with wearables-lessons learned from a machine learning challenge", *IEEE access*, 2021, **9**, 103325-103336.

9. Tine Kolenik, Matjaž Gams, "Persuasive technology for mental health: one step closer to (mental health care) equality?", *IEEE technology & society magazine*, 2021, **40**, 1, 80-86.

10. Vito Janko, Gašper Slapničar, Erik Dovgan, Nina Reščič, Tine Kolenik, Martin Gjoreski, Maj Smerkol, Matjaž Gams, Mitja Luštrek, "Machine learning for analyzing non-countermeasure factors affecting early spread of COVID-19", *International journal of environmental research and public health*, 2021, **18**, 13, 6750.

11. Marija Dragojlović, Igor Milanović, Anton Gradišek, Sandra V. Kurko, Miodrag Mitrić, Anja Umićević, Jana Radaković, Katarina Batalović, "Mechanochemical modification of LiAlH$_4$ with Fe$_2$O$_3$: a combined DFT and experimental study", *International journal of hydrogen energy*, 2021, **46**, 24, 13070-13081.

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13. Anton Gradišek, Mario Cifelli, Donatella Ancora, Ana Sepe, Boštjan Zalar, Tomaž Apih, Valentina Domenici, "Analysis of extra virgin olive oils from two italian regions by means of proton nuclear magnetic resonance relaxation and relaxometry measurements", *Journal of agricultural and food chemistry*, 2021, **69**, 41, 12073-12080.

14. Donatella Ancora, Jerneja Milavec, Anton Gradišek, Mario Cifelli, Ana Sepe, Tomaž Apih, Boštjan Zalar, Valentina Domenici, "Sensitivity of proton NMR relaxation and proton nmr diffusion measurements to olive oil adulterations with vegetable oils", *Journal of agricultural and food chemistry*, 2021, **69**, 41, 12081-12088.

15. Luka Pirker *et al.* (11 authors), "Sterilization of polypropylene membranes of facepiece respirators by ionizing radiation", *Journal of membrane science*, 2021, **619**, 118756.

16. Anton Gradišek, Mathias S. Jørgensen, Mark Paskevicius, Bjarne R. S. Hansen, Torben R. Jensen, "Molecular dynamics in Ag$_2$B$_{12}$H$_{12}$ studied by nuclear magnetic resonance", *The journal of physical chemistry. C, Nanomaterials and interfaces*, 2021, **125**, 10, 5534-5541.

17. Valentin Koblar, Bogdan Filipič, "Evolutionary design of a system for online surface roughness measurements", *Mathematics*, 2021, **9**, 16, 1904.

18. Nikolaus Hansen, Anne Auger, Raymond Ros, Olaf Mersmann, Tea Tušar, Dimo Brockhoff, "COCO: a platform for comparing continuous optimizers in a black-box setting", *Optimization methods & software*, 2021, **36**, 1, 114-144.

19. Svjetlana Fajfer, David Susič, "Colored scalar mediated nucleon decays to an invisible fermion", *Physical review. D*, 2021, **103**, 5, 055012.

20. Els Clays *et al.* (21 authors), "Proof-of-concept trial results of the HeartMan mobile personal health system for self-management in congestive heart failure", *Scientific reports*, 2021, **11**, 5663.

21. Vito Janko, Mitja Luštrek, "A general framework for making context-recognition systems more energy efficient", *Sensors*, 2021, **21**, 3, 766.

22. Anja Pogačnik Krajnc, Luka Pirker, Urška Gradišar Centa, Anton Gradišek, Igor B. Mekjavić, Matej Godnič, Metod Čebašek, Tina Bregant, Maja Remškar, "Size- and time-dependent particle removal efficiency of face masks and improvised respiratory protection equipment used during the COVID-19 pandemic", *Sensors*, 2021, **21**, 5, 1567.

23. Gašper Slapničar, Wenjin Wang, Mitja Luštrek, "Classification of hemodynamics scenarios from a public radar dataset using a deep learning approach", *Sensors*, 2021, **21**, 5, 1836.

24. Simon Stankoski, Marko Jordan, Hristijan Gjoreski, Mitja Luštrek, "Smartwatch-based eating detection: data selection for machine learning from imbalanced data with imperfect labels", *Sensors*, 2021, **21**, 5, 1902.

25. Hans-Peter Schöner, Paolo Pretto, Jaka Sodnik, Boštjan Kaluža, Mojca Komavec, Damir Varešanović, Hanna Chouchane, Jacobo Antona-Makoshi, "A safety score for the assessment of driving style", *Traffic injury prevention*, 2021, **22**, 5, 384-389.

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Review Article

1. Lina Badimon *et al.* (19 authors), on behalf of EU-CardioRNA COSTAction CA17129, "Cardiovascular RNA markers and artificial intelligence may improve COVID-19 outcome: a position paper from the EU-CardioRNA COST Action CA17129", *Cardiovascular Research*, 2021, **117**, 8, 1823-1840.

2. Matjaž Gams, Tine Kolenik, "Relations between electronics, artificial intelligence and information society through information society rules", *Electronics*, 2021, **10**, 4, 514.

3. Tine Kolenik, Matjaž Gams, "Intelligent cognitive assistants for attitude and behavior change support in mental health: state-of-the-art technical review", *Electronics*, 2021, **10**, 11, 1250.

Published Conference Contribution

1. Aljoša Vodopija, Beate Breiderhoff, Boris Naujoks, Bogdan Filipič, "Design of cyclone dust separators: a constrained multiobjective optimization perspective", In: *2021 IEEE Congress on Evolutionary Computation (CEC), June 28th-July 1st 2021, Kraków, Poland*, IEEE, 2021, 1983-1990.

2. Amadej Jankovič, Tine Kolenik, Veljko Pejović, "Mobilna osebnostno-prilagojena aplikacija za spodbujanje pozitivne spremembe vedenja", In: *28. Dnevi slovenske informatike, Portorož, 19.-20. 10. 2021*, Digitalizacija: uspešneje, hitreje, ceneje, Slovensko društvo Informatika, 2021, 105-115.

3. Amadej Jankovič, Tine Kolenik, Veljko Pejović, "The role of personality-tailored notifications in mobile-based behavior change intervention", In: *HCI-SI 2021, 6th Human-Computer Interaction Slovenia Conference, Koper, Slovenia, November 8 2021*, Proceedings, (CEUR Workshop Proceedings **3054**), CEUR-WS, 2021, 18-22.

4. Tine Kolenik, Matjaž Gams, "Increasing mental health care access with persuasive technology for social good", In: *IJCAI 2020 AI for Social Good Workshop, January 7-8 2021*, Center for Research on Computation and Society, 2021.

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6. Carlo De Masi, Simon Stankoski, Vincent Cergolj, Mitja Luštrek, "Intent recognition and drinking detection for assisting kitchen-based activities", In: *IS 2021, Slovenian Conference on Artificial Intelligence, 8. October 2021, Ljubljana, Slovenia*, Proceedings of the 24th International Multiconference Information Society, volume A, Institut "Jožef Stefan", 2021, 15-18.

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15. Klemen Bele, Erik Dovgan, Primož Kocuvan, Matjaž Gams, "Description of health service selection and structure of ISE-EMH program", In: *IS 2021, Insieme Project Workshop, 5. October 2021, Ljubljana, Slovenia*, Proceedings of the 24th International Multiconference Information Society, volume D, Institut "Jožef Stefan", 2021, 23-26.

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22. Erik Dovgan, Maj Smerkol, Miljana Sulajkovska, Matjaž Gams, "Supporting decision-making in the urban mobility policy making", In: *IS 2021, URBANITE Workshop 2021, 8 October 2021, Ljubljana, Slovenia*, Proceedings of the 24th International Multiconference Information Society, volume H, Institut "Jožef Stefan", 2021, 28-31.

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31. Nina Reščič *et al.* (12 authors), "Finding efficient intervention plans against Covid-19: second place at the XPRIZE Pandemic Response Challenge", In: *ETAI 2021, XV International Conference, September 23-24 2021*, Proceedings, (ETAI Megunarodna Konferencija **1** 2), 2021, 139-143.

32. Matjaž Gams, "Is web transforming our minds and where is our civilisation going to?", In: *ETAI 2021, XV International Conference, September 23-24 2021*, Proceedings, (ETAI Megunarodna Konferencija **1** 2), 2021, 153-156.

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INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Clement Picard, Vito Janko, Nina Reščič, Martin Gjoreski, Mitja Luštrek, "Identification of cooking preparation using motion capture data: a submission to the cooking activity recognition challenge", In: *Human activity recognition challenge*, (Smart innovation, systems and technologies **199**), Springer, 2021, 103-113.

2. Junoš Lukan, Gregor Geršak, "Predicting task difficulty through psychophysiology", In: *Applying bio-measurements methodologies in science education research*, Springer, 2021, 55-70.

SCIENTIFIC MONOGRAPH

1. Jana Krivec, *Improve your life by playing a game: learn how to turn your life activities into lifelong skills!*, Thinkers Publishing, 2021.

PATENT

1. Jaka Sodnik, Boštjan Kaluža, Mojca Komavec, Kristina Stojmenova, *A driver evaluation procedure and the device for carrying out the procedure*, SI25874 (A), Urad RS za intelektualno lastnino, 29. 01. 2021.

The Department of Reactor Engineering is involved in basic and applied research in the fields of nuclear engineering and safety. Topics include the theoretical and experimental research of basic thermal-hydrodynamic phenomena, thermal-hydraulic safety analyses of fission and fusion reactors, and structural safety analyses. Most research activities are part of international cooperation programmes. Research results are incorporated into projects for industry and for the regulatory authority, as well as into undergraduate and doctoral studies programmes. The department also continued with the modelling of the COVID-19 epidemic development in Slovenia by applying methods from nuclear energy.

Head:
Prof. Leon Cizelj

Modelling of basic thermal-hydrodynamic phenomena

In the field of two-phase gas-liquid flow research, we simulated Taylor bubbles (bullet-shaped bubbles that extend over almost the entire tube cross-section) in the counter-current turbulent-flow regime using the OpenFoam open-source Computational Fluid Dynamics (CFD) code. The volume of fluid (VOF) method was used together with large eddy simulations (LES), which allows a high-fidelity reproduction of the flow. The results were validated using measurements obtained in our own THELMA laboratory. Since simulations overestimate the Taylor-bubble decay rate by about one-to-two orders of magnitude, new models are being developed for more accurate interface reconstruction as well as bubble break-up and coalescence in the wake of Taylor bubbles.

The development of advanced simulation tools for multiphase flows using the OpenFoam library was continued. We simulated an isothermal counter-current stratified flow in the channel of the WENKA (Water Entrainment Channel Karlsruhe, Germany) experiment using a hybrid-morphology-adaptive two-fluid model extended with a turbulence-damping model near the interface. Two damping strategies were investigated: symmetric, with damping in both phases, and asymmetric, with damping only in the gas phase. The comparison shows that the asymmetric approach offers an improved prediction of the turbulent kinetic energy on the liquid side of the interface, but at a cost of diminished accuracy of the predicted velocity profiles on the gas side. The research is being carried out within the CROSSING project in cooperation with Helmholtz-Zentrum Dresden-Rossendorf (Germany).

The basic phenomena of vapour explosion and debris bed coolability, which might occur during a severe accident if hot reactor-core melt comes into contact with coolant, were further investigated. Among studies of vapour explosions in stratified melt-coolant configurations, the PULiMS and SES experiments (both performed at the Royal Institute of Technology, Sweden) were simulated, using the developed model of the premixing layer's formation, implemented in our patch of the MC3D code (Institut de radioprotection et de sûreté nucléaire - IRSN, France). While the premixed layer of melt drops in the coolant layer seems adequately simulated, the comparison of experiments and simulations indicates potential contributions to the melt-coolant mixing (apart from the premixed layer) also from fragmentation of the melt jet and mixing during the explosion itself. Next, to improve the understanding of heat transfer during the explosion phase, CFD simulations of the film boiling TR-EPAM experiments (Commissariat à l'énergie atomique et aux énergies alternatives - CEA, France) were restarted. We have also started investigations of debris bed coolability in top flooding conditions. A simple one-dimensional analytical model was developed for a basic description of recent debris bed experiments performed in the FLOAT facility (IKE, University of Stuttgart, Germany).

Figure 1: Boiling patterns at refrigerant mass flux 300 kg/m²s and different surface heat fluxes (recorded with a high-speed camera at 200 fps).

In the field of hydrogen distribution in nuclear power plant (NPP) containment, simulations of atmosphere stratification (in the sense of composition) erosion using a vertical jet, performed in the PANDA (Paul Scherrer Institute, Switzerland) and SPARC (Korea Atomic Energy Research Institute) experimental facilities were continued. A model with dynamic Prandtl and Schmidt numbers was proposed, which represents an extension of existing modelling to conditions that may be expected during a severe accident following reactor core oxydation and hydrogen release into the containment.
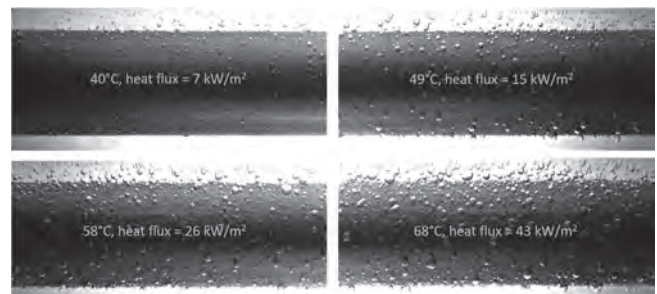
Experimental investigations in THELMA laboratory

In the Thermal-Hydraulics Experimental Laboratory for Multiphase Applications (THELMA) we continued flow-boiling experiments in a test section that represents part of a single rod in a light-water nuclear reactor fuel assembly. New experiments were performed in the horizontal orientation of the section. Flow boiling was investigated using a high-speed camera at constant flow rates and varying heating power at the wall. The obtained images were post-processed for the first time with a machine-learning technique and artificial neural networks, which provided information on the bubble-size distribution. Heat transfer in the test section was further studied and optimized using a series of single-phase CFD simulations, which involved primary and secondary fluid of similar (isothermal) and different (non-isothermal) temperatures.

In the Taylor-bubble experiment the liquid velocity field was measured using the Particle Image Velocimetry (PIV) technique. Due to the high reflection of laser light on the bubble interface, the Laser Induced Fluorescence technique was applied, which uses fluorescent tracking particles that glow at a different wavelength than laser light.

In the Taylor-bubble experiment, the velocity was measured using the Particle Image Velocimetry technique.

In this way, the sensitive sensor of the high-speed camera can be protected with a filter that does not transmit laser light. The obtained images were processed with programmes that reproduce the velocity field of the liquid phase. For single-phase turbulent flow in a pipe, we studied the influence of seeding particles type and concentration (density) on the accuracy of the obtained velocity fields. Bubble-decay-rate measurements are used for the validation of Taylor-bubble simulations in a counter-current turbulent flow regime (mentioned earlier).

We continued the study of temperature perturbations from turbulent coolant flow to an adjacent heated wall. In this experimental rig, a fully developed turbulent flow in a rectangular duct was heated with a thin metal foil flush with the wall and powered with DC current. Temperature turbulent fluctuations at different Reynolds and Prandtl fluid numbers were observed on the outer side of the foil using a high-speed infra-red camera. Additional LES simulations that were performed, which took into account heat conduction in the heated wall together with the convective heat transfer in the fluid, i.e. conjugate heat-transfer simulations, further improved our predictions of the power spectra of temperature fluctuations on the heated foil.

Thermal-hydraulic safety analyses of fission and fusion reactors

BETHSY (CEA) is an integral test facility that was designed to simulate pressurized water reactor (PWR) accidents. The BETHSY 9.1b experiment represents a 2" small break loss-of-coolant accident with loss of a high-pressure injection system (after the Fukushima-Daiichi nuclear accident in Japan in 2011, this type of accident is considered as part of Design Extension Conditions, category A), so that a delayed operator action for secondary system depressurization was performed. The experiment was simulated with the TRACE advanced thermal-hydraulic system code, and the simulation results were compared to experimental ones.

The European project AMHYCO deals with the prevention of hydrogen and carbon monoxyde combustion in an NPP containment during a severe accident. With the system code MELCOR, three possible station blackout scenarios in a two-loop PWR with different cold leg break sizes were simulated, with the purpose to provide hydrogen sources for further analyses of ensuing phenomena in the containment.

The assessment of the thermal loading of the DEMO fusion reactor breeding blanket (BB) during an ex-vessel loss-of-coolant accident was continued. The numerical model was updated by considering a refined decay heat generated inside the BB and new transient simulations were performed to re-evaluate the cooling performance and temperature distribution of passive in-vessel components due to in-vessel natural convection of injected gas under refined conditions. The CFD simulations are supported with the prediction of a lumped-parameter model, which is used for fast predictions of longer transients. The work was performed in the frame of the European nuclear fusion project WPDES.

We have upgraded a calorimeter design for the Neutral Beam Injector (NBI) of the Divertor Tokamak Test facility (DTT), which is a new tokamak to be constructed in Frascati (Italy). The calorimeter is designed as a movable panel with cooling U-tubes equipped with swirl tape inserts. The new calorimeter design considers increased beam power and a significantly changed overall NBI design. Design changes required re-calculation of ther-
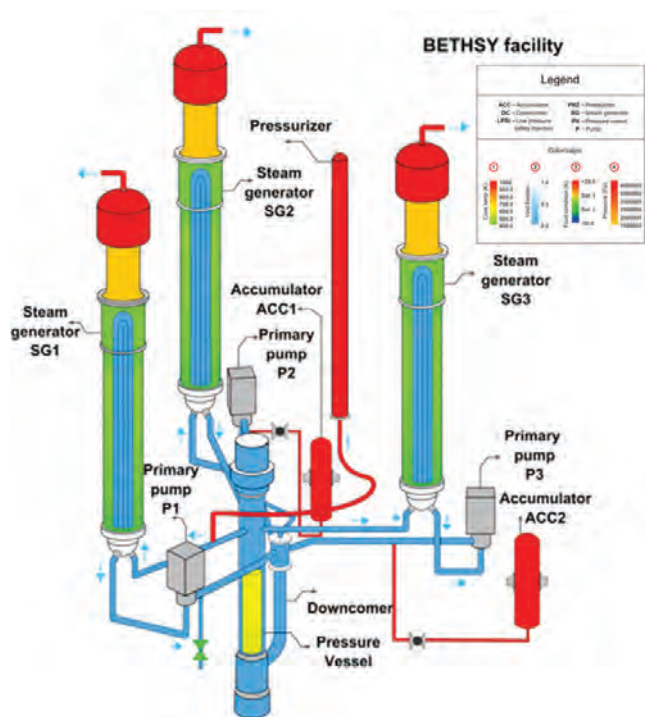

Figure 2: Animation model of BETHSY facility (CEA, France).

mal heat loads and the temperature distribution in the calorimeter. The work was performed in cooperation with Consorzio RFX (Italy).

A water-cooled divertor element for stellarator W7-X, located in Greifswald (Germany), is being developed within the European fusion project DIV. Our group performed a CFD analysis of a prototype divertor element. A single-fluid modelling approach was used to simulate the cooling water flow and its effect on the wall-temperature distribution of the cooling channel. Preliminary results have shown that the temperatures of the cooling-element structures are below the critical values for the anticipated heat loads and operating conditions.

The thermal loading of the DEMO fusion reactor breeding blanket during an ex-vessel loss-of-coolant accident was evaluated.

Structural safety analyses

Research activities focused on the process of intergranular stress-corrosion cracking, in particular on the micromechanical aspects of its initiation stage. In a study conducted in cooperation with CEA, grain boundaries were assigned to different grain-boundary types based on their associated strengths. A new parameter was identified that suffices for quantifying intergranular normal stress fluctuations on a particular grain-boundary type.

The obtained results initiated a highly ambitious follow-up project, with the goal to construct a simple analytical model for predicting local grain-boundary stresses in an arbitrary polycrystalline material, on any grain-boundary type and for any applied loading. We managed to decouple the effect of loading from the contribution of grain-boundary type and of the material used. A simplified model scenario based on a bi-crystal model

We are developing an analytical model for predicting local grain-boundary stresses in an arbitrary polycrystalline material, on any grain-boundary type and for any applied loading.

embedded in a homogenous elastic medium was proposed and Reuss and Voigt limits were applied at different length scales. The results have been verified by finite-element simulations and show some very promising prospects.

Within the European project ATLAS+ our activities were continued with the goal to develop improved methods for evaluating fatigue-crack growth caused by flow mixing. Structural models of a T-junction piping containing cracks were developed and then employed in subsequent thermo-mechanical and fracture-mechanics analyses.

Preliminary analyses of a two-loop PWR under selected loss-of-coolant-accident (LOCA) scenarios were performed in the frame of pressurized thermal shock (PTS) studies. Thermal-hydraulic and structural analyses were carried out, respectively, with RELAP5 and FAVOR computer codes. Available shifts of the ductile-to-brittle (reference) temperature of the reactor pressure vessel's material were compared to existing regulatory limits.

Within the European project APAL, the review activities related to state-of-the-art methods and national experience on PTS were finalized and a small-break LOCA was selected as the "base case" scenario for follow-up studies.

Thermo-mechanical analyses of a dry cask for nuclear spent-fuel storage were carried out in cooperation with the Polytechnic University of Madrid (Spain) using available cask temperatures obtained in CFD simulations.

Referring to the already-mentioned tokamak to be constructed in Frascati (Italy), thermo-mechanical analyses using thermal loads from CFD simulations were performed to further evaluate the deformations and stresses of the calorimeter conceptual design for the Neutral Beam Injector.

Modelling of the COVID-19 epidemic's development in Slovenia

As the equations for the spreading of infections are similar to the equations of the chain reaction in a nuclear reactor, the department was involved in the prediction of the COVID-19 epidemic progression. The SEIR (Susceptible, Exposed, Infectious, Recovered) model was fitted with publicly available data and the impact of the population's response to the measures could also be taken into account.

We consider in an integral way most of the available data, such as: number of confirmed cases, number of people hospitalized and in intensive care units, number of deceased people, as well as the age structures. Immunisation and vaccination are taken into account as well. We treat four different courses of the disease and calculate nine specific reproductive numbers of the spread of the infection, on the basis of which the epidemic trend is determined. We check the initial part of the prognosis with what is already in the "waiting room", i.e., the known number of confirmed cases in the last period by age categories, who will, with a certain time lag and probability,

Figure 3: Projection of the number of hospitalized COVID-19 patients in intensive-care units.

appear in hospitals, intensive care units and finally die. We also take into account soft data, i.e., non-quantitative information, such as that an infection has entered a home for the elderly and thus an outbreak with a specific age structure has occurred.

For the government's expert advisory group, we have been preparing daily analyses of the epidemic's situation and prognoses of the number of hospitalized people.

For the Government of Slovenia's expert advisory group, we prepared daily analyses of the epidemic situation and prognoses of the number of hospitalized and deceased people, and estimates of the reproductive number of infections R (which must be below one for the epidemic to be contained). The results of our analyses and the prognoses were regularly published.

Technical cooperation, consulting services and education

In 2021 the Reactor Engineering Division cooperated in projects for industry as well. As an authorized institution for radiation and nuclear safety, we prepared an independent evaluation on outage and refueling activities in the Krško NPP. We performed the review of safety factors in the subject area of safety analyses within the Krško NPP Third Periodic Safety Review. For the Slovenian Nuclear Safety Administration, we analysed the influence of design extension conditions' equipment on severe accident development in the same NPP using the MELCOR severe accidents code.

Researchers at the department represent the core staff of the Chair for nuclear engineering at the Faculty of Mathematics and Physics at the University of Ljubljana, and are involved in nuclear engineering undergraduate, master's and doctoral studies. The programmes are associated with the European Nuclear Education Network (ENEN). In the autumn of 2021, the second generation of students of the international MSc programme in nuclear engineering SARENA, in which the department is actively involved, was admitted to the faculty.

Awards and appointments

1. Janez Kokalj, Matjaž Leskovar, Mitja Uršič: Best Technical Track Paper (ENYGF Conference, Tarragona, Spain) Jóvenes Nucleares, Sociedad Nuclear Española and ENS YGN, "Model for premixed layer formation in stratified fuel-coolant configuration and its application"
2. Mihael Boštjan Končar, Matej Tekavčič, Mitja Uršič: Young Author Award (International Conference Nuclear Energy for New Europe 2021, Portorož, Slovenia) Nuclear Society of Slovenia, "Film boiling simulation around cylinder with ANSYS Fluent"
3. Jan Kren: Best Paper by a Young Researcher Award (Symposium on Advances in Computational Heat Transfer-21, virtual) International Centre for Heat and Mass Transfer, "Numerical analysis of turbulent heat transfer in rectangular duct"

Organization of conferences, congresses and meetings

1. Young Generation Nuclear Conference, 19. 5. 2021 (virtual)
2. International Conference Nuclear Energy for New Europe 2021, Portorož, Slovenia, 6.-9. 9. 2021
3. U.S. - SLO Nuclear Innovation Workshop, JSI Reactor center, 18.-19. 10. 2021

INTERNATIONAL PROJECTS

1. H2020 - ATLASplus; Advanced Structural Integrity Assessment Tools for Safe Long Term Operation
Prof. Leon Cizelj
European Commission
2. H2020 - NARSIS; New Approach to Reactor Safety Improvements
Dr. Andrej Prošek
European Commission
3. H2020 - ENENplus; Attract, Retain and Develop New Nuclear Talents Beyond Academic Curricula
Asst. Prof. Ivo Kljenak
European Commission
4. H2020 - PIACE; Passive Isolation Condenser
Asst. Prof. Ivo Kljenak
European Commission
5. H2020 - sCO2-4-NPP; Innovative sCO2-Based Heat Removal Technology for an Increased Level of Safety of Nuclear Power Plants
Dr. Andrej Prošek
Electricite de France S.a.
6. H2020 - EURAD; European Joint Programme on Radioactive Waste Management
Prof. Leon Cizelj
European Commission
7. H2020 - ECC-SMART; Joint European Canadian Chinese Development of Small Modular Reactor Technology
Prof. Leon Cizelj
European Commission
8. H2020 - AMHYCO; Towards an Enhanced Accident Management of the Hydrogen/CO Combustion Risk
Asst. Prof. Ivo Kljenak
European Commission
9. H2020 - APAL; Advanced PTS Analysis for LTO
Dr. Oriol Costa Garrido
European Commission
10. H2020 - EUROfusion; Research Unit - Administration and Services RU – FU
Asst. Prof. Boštjan Končar
European Commission
11. HE - EUROfusion; WP12: DIV_HE-FU
Asst. Prof. Boštjan Končar
European Commission
12. HE - EUROfusion; WP08: DES-1,2_HE-FU
Dr. Martin Draksler
European Commission
13. HE - EUROfusion; WP19: SAE-1_HE-FU
Dr. Mitja Uršič
European Commission
14. HE - EUROfusion; WP25: PMU_HE-FU, RU-Mgmt-1_HE-FU
Asst. Prof. Boštjan Končar
European Commission
15. HE - EUROfusion; WP24: TRED_HE-FU, EDU_HE-FU
Asst. Prof. Boštjan Končar
European Commission

RESEARCH PROGRAMMES

1. Reactor engineering
   Prof. Leon Cizelj
2. Fusion technologies
   Asst. Prof. Boštjan Končar

R&D GRANTS AND CONTRACTS

1. Efficient cooling concepts for high heat flux components in fusion reactor
   Asst. Prof. Boštjan Končar
2. Investigation of turbulent heat transfer in an annulus through advanced experimental and computational methods
   Prof. Iztok Tiselj
3. Simulation of selected design extension conditions without core melt
   Asst. Prof. Boštjan Končar
4. Understanding stratified steam explosions in reactor conditions
   Dr. Matjaž Leskovar

NEW CONTRACTS

1. Joint Expert Assessment of the Outage Activities, Interventions and Tests during a shutdown and refueling outage 2021
   Dr. Mitja Uršič
   Elektroinštitut Milan Vidmar
2. Analysis of Influence of DEC Equipment on Severe Accident Development in Krško NPP with MELCOR code
   Dr. Matjaž Leskovar
   Ministry of the Environment and Spatial Planning
3. Cooperation in an international CAMP and CSARP program
   Dr. Andrej Prošek
   Krško Nuclear Power Plant
4. Investigation of turbulent heat transfer in an annulus through advanced experimental and computational methods
   Prof. Iztok Tiselj
   Krško Nuclear Power Plant
5. Simulation of selected design extension conditions without core melt
   Asst. Prof. Boštjan Končar
   Krško Nuclear Power Plant
6. Understanding stratified steam explosions in reactor conditions
   Dr. Matjaž Leskovar
   Krško Nuclear Power Plant
7. NEK PSR3 Project Task „Safety Analyses"
   Dr. Mitja Uršič
   Krško Nuclear Power Plant

VISITORS FROM ABROAD

1. Mr. Onejin Wu and Mr. Matjaž Kavčič, Embassy of the United States, Ljubljana, Slovenia, 2. 7. 2021

STAFF

Researchers
1. **Prof. Leon Cizelj, Head**
2. Dr. Oriol Costa Garrido
3. Dr. Martin Draksler
4. Dr. Samir El Shawish
5. Asst. Prof. Ivo Kljenak
6. Asst. Prof. Boštjan Končar
7. Dr. Matjaž Leskovar
8. Dr. Blaž Mikuž
9. Dr. Andrej Prošek
10. Dr. Mohit Pramod Sharma
11. Prof. Iztok Tiselj
12. Dr. Mitja Uršič
Postdoctoral associates
13. Dr. Timon Mede
14. *Dr. Jure Oder, on leave since 01.02.21*

15. Dr. Matej Tekavčič
Postgraduates
16. Dr. Janez Kokalj
17. Jan Kren, B. Sc.
18. Rok Krpan, B. Sc.
19. Matic Kunšek, B. Sc.
20. *Nikola Veljanovski, M. Sc., left 01.06.21*
21. Boštjan Zajec, B. Sc.
Technical officers
22. Anil Kumar Basavaraj, B. Sc.
23. *Sandi Cimerman, B. Sc., left 07.05.21*
24. Andrej Sušnik, B. Sc.
Technical and administrative staff
25. Tanja Klopčič
26. Zoran Petrič, B. Sc.
27. Nina Rehar, B. Sc.

BIBLIOGRAPHY

Original Article

1. Ulrich Bieder, Heleen Uitslag-Doolaard, Blaž Mikuž, "Investigation of pressure loss and velocity distribution in fuel assemblies with wire-wrapped rods by using RANS and LES with wall functions", *Annals of Nuclear Energy*, 2021, **152**, 108025.
2. Jure Oder, Cedric Flageul, Iztok Tiselj, "Statistical uncertainty of DNS in geometries without homogeneous directions", *Applied sciences*, 2021, **11**, 4, 1399.
3. Boštjan Zajec, Marko Matkovič, Nejc Kosanič, Jure Oder, Blaž Mikuž, Jan Kren, Iztok Tiselj, "Turbulent flow over confined backward-facing step: PIV vs. DNS", *Applied sciences*, 2021, **11**, 22, 10582.
4. Samir El Shawish, Timon Mede, Jeremy Hure, "A single grain boundary parameter to characterize normal stress fluctuations in materials with elastic cubic grains", *European journal of mechanics. A, Solids*, 2021, **89**, 104293.
5. Louis Giannone, Samir El Shawish, Albrecht Herrmann, Arne Kallenbach, K.-H. Schuhbeck, George Vayakis, Christopher Watts, Irene Zammuto, "Shunt and Rogowski coil measurements on ASDEX upgrade in support of DEMO detachment control", *Fusion engineering and design*, 2021, **166**, 112276.
6. Boštjan Končar, Domen Ovtar, Oriol Costa Garrido, Piero Agostinetti, "Calorimeter conceptual design for Neutral Beam Injector of DTT - CFD optimisation and thermal stress analysis", *Fusion engineering and design*, 2021, **170**, 112469.
7. Martin Draksler, Christian Bachmann, Boštjan Končar, "Assessment of residual heat removal from activated breeding blanket segment during remote handling in DEMO", *Fusion engineering and design*, 2021, **173**, 112891.
8. Iztok Tiselj, Mohit Sharma, Boštjan Zajec, Nikola Veljanovski, Jan Kren, Leon Cizelj, Blaž Mikuž, "Investigation of turbulent flow in square duct with heated foil thermometry", *International journal of heat and mass transfer*, 2021, **175**, 121381.
9. Mohit Sharma, A. Moharana, "Simulation of turbulent mixing rate in simulated subchannels of a reactor rod bundle", *Kerntechnik*, 2021, **86**, 3, 210-216.

10. Janez Kokalj, Mitja Uršič, Matjaž Leskovar, "Modelling of premixed layer formation in stratified fuel-coolant configuration", *Nuclear Engineering and Design*, 2021, **378**, 111261.
11. Matej Tekavčič, Richard Meller, Fabian Schlegel, "Validation of a morphology adaptive multi-field two-fluid model considering counter-current stratified flow with interfacial turbulence damping", *Nuclear Engineering and Design*, 2021, **379**, 111223.
12. Rok Krpan, Iztok Tiselj, Ivo Kljenak, "Simulations of PANDA and SPARC experiments on containment atmosphere mixing caused by vertical gas injection", *Nuclear Engineering and Design*, 2021, **384**, 111464.
13. Julio Benavides Rodríguez, Oriol Costa Garrido, Gonzalo Jiménez, Leon Cizelj, "Thermo-mechanical analysis of a nuclear spent fuel dry cask using CFD results in a FE code", *Nuclear Engineering and Design*, 2021, **384**, 111481.

PUBLISHED CONFERENCE CONTRIBUTION

1. Petra Fic *et al.* (12 authors), "COVID-19 vigilance: towards better risk assessment and communication during the next wave", In: *40th International Conference on Organizational Science Development: values, competencies and changes in organizations, 17-19 March 2021*, Conference Proceedings, University of Maribor, 2021, 199-217.
2. Boštjan Zajec, Boštjan Končar, Leon Cizelj, "Visualization and void distribution analysis in flow boiling of R245fa in horizontal annulus", In: *ATE-HEFAT 2021, 15th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics, 26-28 July 2021*, American Society of Thermal and Fluids Engineers, 2021, 2319-2339.
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REACTOR INFRASTRUCTURE CENTRE RIC

The Reactor Infrastructure Centre (RIC) incorporates a TRIGA Mark II research reactor and a Hot-Cells Facility. The reactor, operating since 1966, is used for neutron research, education and training, and radioactive isotope production. A detailed technical description of the reactor is available at ric.ijs.si/en/. The Hot-Cells Facility is used for the treatment and handling of radioactive materials and radioactive waste, for both research and applicative projects. In addition, it is used for performing regular radiological measurements of radioactive waste and irradiated samples.

Members of the reactor staff operate and maintain the reactor. They also participate in other activities, requiring specialists skilled in working with sources of radiation and in reactor technology, such as servicing of industrial radioactive sources, surveillance of fuel management in NPP Krško, and characterization, processing, and preparation of radioactive waste.

Head:
Prof. Borut Smodiš

In 2021 the reactor operated for 167 days (739 hours) and produced 128.2 MWh of heat. Altogether, 70 pulses were carried out and 641 samples were irradiated in the irradiation channels. The reactor operated almost twice as much as the year when the Covid-19 pandemic hit, and at the largest capacity in the last decade. With the exception of 2020, an upwards trend has been observed since 2015 in all operational indicators, which only confirms our centre's success.

The reactor's operators supported users by performing operations and services for which the users were not qualified and authorized, such as operating the reactor, performing irradiations and experiments, and handling irradiated samples.

In 2021 the TRIGA Mark II reactor was mainly used as a neutron source for research in different areas, such as radiation-hardness studies, neutron-activation analysis, education, and training. For educational purposes, it was mostly used by the Reactor Physics Department (F8), while the Nuclear Training Centre (ICJT in Slovene) used it for training purposes, and the Department of Environmental Sciences (O2) and the Department of Experimental Particles Physics (F9) both used it for sample irradiation. Lastly, the reactor was used for experiments in reactor physics by the Reactor Physics Department (F8). The shutdown reactor, being a powerful source of gamma radiation, was used for testing the resistance of electronic components and other materials to radiation. In the Hot-Cells Facility, the activities were mostly performed by the Department of Environmental Sciences (O2), the Radiation Protection Unit – RPU (SVPIS in Slovene) and the Slovenian Agency for Radioactive Waste Management (ARAO) – processing and preparation of radioactive waste for storage.

Figure 1: Neutron-flux-mapping exercise for the students from Aix Marseille University (remote).

Figure 2: CEA and JSI researchers performing calorimetry experiments at TRIGA.

The reactor was used for the following research activities:
– Reactor physics and neutronics.
– Activation analysis.
– Research on the radiation damage of semiconductors.
– Neutron dosimetry and spectrometry.
– Activation of materials, nuclear waste, and decommissioning.
– Radiation-hardness studies.
– Irradiation of materials for fusion reactors.
– Irradiation of electronic components.
– Irradiation of 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.

Figure 3: Modified reactor-core configuration.

Figure 4: SARENA project participants sitting in on practical classes, provided in English by researchers of the Reactor Physics Department (F8) and the reactor operators.

Figure 5: University of Uppsala students getting familiar with reactor operations.

In January a cycle of practical classes for master's students at the Faculty of Mathematics and Physics, University of Ljubljana was completed. It was mostly carried out remotely. During the lockdown the classes had to be adapted accordingly. Now, the students and course participants can manipulate our measuring instruments remotely, from any part of the world. We are, therefore, available even to those who previously could not afford to travel to Slovenia.

In February and November, FT-TIMS samples were irradiated for CEA. Each sample must be irradiated for 20 hours, at full power. The samples were irradiated in a modified thermal column, with the ratio 500:1 of thermal neutron flux versus the total.

In March and April the reactor was a preparation site for start-up tests at the Krško NPP. The Reactor Physics Department (F8) used the TRIGA reactor for testing and calibration of their instruments before performing start-up tests at the Krško NPP. The latter was able to operate at full power after the tests were performed.

In April a short campaign of pulse operation with the intention of characterising a Cherenkov detector was carried out. The detector was first used in May for a new practical class for the students of the Faculty of Mathematics and Physics.

Besides the aforementioned class with the Cherenkov detector, another class took place in May for students of the Faculty of Mathematics and Physics, with a self-powered neutron detector. No external power is required for this kind of detector as it is powered by irradiation. It is a fairly new piece of technology that can be used in nuclear power plants, in the case of a power outage that could cause a serious accident.

Before summer, the reactor's core configuration was modified. Six fresh fuel elements were added. The old triangular channel was replaced with a new one, with the addition of another triangular channel. The modified reactor core is expected to remain unchanged for the next few years.

In July a three-day course was carried out remotely for the students of Aix Marseille University.

Calorimetric measurements on different materials were also performed in July, in collaboration with CEA and the Reactor Physics Department (F8).

In September, researchers from Napoli were hosted at our facility to test the neutron-irradiation hardness of their FPGA circuits.

In late September an almost traditional week-long course on experimental reactor physics was organised for the University of Uppsala students.

During the autumn semester, the Faculty of Mathematics and Physics students and the SARENA project participants were hosted at our facility every Monday. The participants came from three different continents and took part in the same practical classes as the Slovenian students. The course was carried out for the first time and the official language was English.

From late October until mid-December, the facility was occupied nearly every afternoon by future reactor operators of the Krško NPP that took part in the Nuclear Power Plant Technologies course, organised by the Milan Čopič Nuclear Training Centre (ICJT).

In early November a short campaign was carried out for CEA and Framatome, in collaboration with the Reactor Physics Department (F8). Its main purpose was to test the SiC detectors' response.

In early December the reactor operators went on a work-related trip to Paris. They visited the Orphe reactor, followed by a three-day visit to the World Nuclear Exhibition, which is the largest nuclear fair in our region and is organised every two years.

In December the reactor was mainly operated in pulse mode, due to the short pulse campaign in collaboration with CEA and Instrumentation Technologies (a Slovenian company from Solkan), the Faculty of Mathematics and Physics students' course and the Politecnico di Milano students' course.

Throughout the entire year many detectors for CERN and other large particle accelerators were irradiated, in collaboration with the Department of Experimental Particle Physics (F9), or directly for the contractor.

Collaboration with the company DITO, which develops and sells the best radiation-resistant lighting, continued in 2021. Specific lighting components were irradiated to decide their levels of radiation hardness.

To keep the spread of the new coronavirus at bay, the number of visitors to the reactor was strictly limited. Open day at the JSI, including the reactor tour, was carried out virtually. In autumn, however, the Reactor Infrastructure Centre took part in the event called European Researchers' Night that enabled in-person visits to the reactor, which was open to visitors in the evening. It was operating at 30-kW power, which is low enough to maintain the visitors' safety, but the Cherenkov radiation, a common indicator of reactor operation, was still visible.

INTERNATIONAL PROJECTS

1. Irradiation Services for the Rolls-Royce Civil Nuclear SAS Company
   Prof. Borut Smodiš
   Rolls-Royce Civil Nuclear SAS
2. H2020 - ENEEP; European Nuclear Experimental Educational Platform
   Prof. Borut Smodiš
   European Commission

R&D GRANTS AND CONTRACTS

1. Irradiations in TRIGA Nuclear Reactor
   Prof. Borut Smodiš

2. Irradiations on the TRIGA Reactor
   Prof. Borut Smodiš
3. Irradiations of FT-TIMS Capsule on the TRIGA Reactor for Years 2020-2022
   Prof. Borut Smodiš
   Cea-Commissariat à l'énergie atomique et aux énergies alternatives
4. Refurbished Lazy Susan
   Prof. Borut Smodiš
   University of Pavia
5. SiC Campaign within the Frame of the Contract between CEA/AMU and FRAMATOME
   Prof. Borut Smodiš
   Cea Saclay

VISITORS FROM ABROAD

1. Dr Robert Bernat, Luka Bakrač, Ruđer Bošković Institute, Zagreb, Croatia, 1-5 March 2021.
2. Clément Barnier, Pierre Vignollet, Stéphane Fargues, Rolls Royce Civil Nuclear SAS, Meylan, France, 23-25 May 2021
3. Loïc Barbot, Gregoire de Izarra, French Alternative Energies and Atomic Energy Commission (CEA) Cadarache, Saint-Paul-lez-Durance, France, 14-15 June 2021.
4. Dr Damien Fourmentel, Hubert Carcreff, French Alternative Energies and Atomic Energy Commission (CEA) Cadarache, Saint-Paul-lez-Durance, France, 19-23 July 2021.
5. Dr Damien Fourmentel, Hubert Carcreff, French Alternative Energies and Atomic Energy Commission (CEA) Cadarache, Saint-Paul-lez-Durance, France, 2-5 November 2021.
6. Dr Laurent Ottaviani, Aix-Marseille University, Marseille, France, 2-5 November 2021.
7. Patrick Konrad, Heiko Jasper, Patrick Weidenauer, Framatome, Saone-et-Loire, France, 2-5 November 2021.
8. Dr Elchin Huseynov, National Nuclear Research Center, Baku, Azerbaijan, 14-28 November 2021.
9. Prof. Stefano Lorenzi, Polytechnic University of Milan, Milan, Italy, 3 December 2021.
10. Loïc Barbot, Gregoire de Izarra, French Alternative Energies and Atomic Energy Commission (CEA) Cadarache, Saint-Paul-lez-Durance, France, 6-10 December 2021.

STAFF

Researcher
1. **Prof. Borut Smodiš**, Head
Postdoctoral associate
2. Dr. Anže Jazbec
Technical and administrative staff
3. Andrej Gyergyek, B. Sc.
4. Jasna Kopač, B. Sc.
5. Marko Rosman
6. Sebastjan Rupnik, B. Sc.
7. Nina Udir, B. Sc.
8. Andraž Verdir, B. Sc.

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PUBLISHED CONFERENCE CONTRIBUTION

1. Jan Malec, Michael Österlund, Andreas Solders, Ali Al-Adili, Anže Jazbec, Sebastjan Rupnik, Vladimir Radulović, Igor Lengar, Luka Snoj, "On teaching experimental reactor physics in times of pandemic", In: *ANIMMA 2021, 7th International Conference on Advancements in Nuclear Instrumentation Measurement Methods and their Applications, 21-25 June 2021, Prague, Czech Republic*, Proceedings, (EPJ web of conferences **253**), 2021, 10001.
2. Vladimir Radulović *et al.* (16 authors), "The European nuclear experimental educational platform – ENEEP: Progress, prospects and

remote education capabilities", In: *ANIMMA 2021, 7th International Conference on Advancements in Nuclear Instrumentation Measurement Methods and their Applications, 21-25 June 2021, Prague, Czech Republic*, Proceedings, (EPJ web of conferences **253**), 2021, 10002.

3. Anže Jazbec, Vladimir Radulović, Sebastjan Rupnik, Borut Smodiš, Luka Snoj, "Jožef Stefan Institute TRIGA research reactor activities in the period from September 2020 – August 2021", In: *NENE 2021, 30th International Conference Nuclear Energy for New Europe, September 6-9, Bled, Slovenia*, Proceedings, Nuclear Society of Slovenia, 2021, 314.

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NETWORKING INFRASTRUCTURE CENTRE

NIC

The Networking Infrastructure Centre (NIC) manages the core network, ICT services and computing infrastructure of the Jožef Stefan Institute. It also supports the development of computing, communication, data and security infrastructure for our research departments, centres and services at the Institute and participates in national and international collaborations.

The NIC's main mission is the administration of computing networks, services and equipment to support the work of users at the Jožef Stefan Institute, their collaborators, projects and research groups, but we also participate in infrastructure-development projects in national and international contexts. We provide for connectivity and integration with local and international communication networks and infrastructures, but we also deliver ICT support for research activities at the Jožef Stefan Institute, including the development, management and administration of the ICT infrastructure, computing facilities and services. NIC is responsible for four main domains: networking infrastructure, network security, network services and distributed network supercomputing.

Head:
Dr. Jan Jona Javoršek

Networking Infrastructure. The Networking Infrastructure Centre maintains and develops the Institute's network backbone as well as departmental networks, wireless networks and dedicated networks for services such as dedicated links to other institutions, secure links to the Reactor Infrastructure Centre Podgorica, connections to high-bandwidth scientific VPN networks through GÉANT and other project support
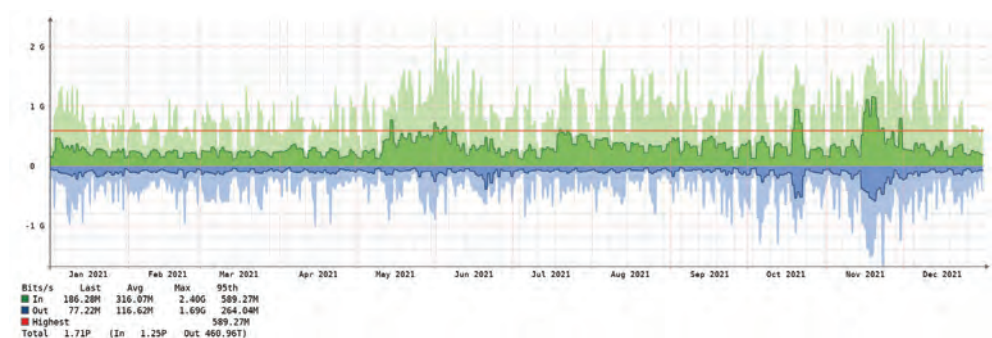
Figure 1: Traffic on the general network was intense throughout the year, while the dedicated networks saw expanded traffic due to new connectivity.

Physical Network: In 2021 we continued extending the capabilities of the physical network as well as updating and upgrading our active equipment, including wireless-access-point installations and core backbone network routers. We expanded the twin 100 Gbit/s connections to Arnes' network to make increased bandwidth available to dedicated supercomputing and storage facilities more accessible. The Institute's backbone network was further optimised, the use of virtual network links for dispersed internal networks, (super)computing clusters and virtual machine farms, including remote VPN access and device-support access for outside contractors, was expanded. We continued to support external connectivity for experiments needing high throughput within projects, such as EuroHOC, EOSC, HPC RIVR, WLCG (Worldwide Large Hadron Collider Computing Grid) for ATLAS, but also Belle2 and other EGI and PRACE using projects over general GÉANT networks and also dedicated scientific VPNs such as LHCONE and PRACE.

Monitoring: Continued expansion of our network requires evolution of our traffic, event and status-monitoring infrastructures well as integration of new monitoring facilities and sensors to capture, monitor, report and react to usage fluctuations and events in our services, security policies, firewalls, authentication and authorization systems, network time systems, e-mail delivery as well as the analysis, processing and security systems themselves, but we also integrate physical room and machine sensory data, environmental data, power-line data, etc.

Wireless network: Thanks to modern, highly efficient components and central control modules we were able to continue to improve wireless coverage and the density of our wireless networks where usage is most condensed.

> **A network with a multi-10 Gbit/s network backbone, modern protocol stacks, a flexible ICT infrastructure supporting numerous fixed and wireless clients has been expanded with fast dedicated external 100 Gbit/s links.**

Network Security. The NIC manages security measures and policies at the external network borderline, in the internal network and regarding the services and software deployments for the users. External network security is implemented with active security devices, firewall systems, secure-first configurations and passive measures (configuration, filtering and supervision). Constant dynamic supervision, traffic monitoring and event analysis is needed to ensure suitable security in the complex constraints and requirements of an open academic network that collide with current security considerations and demands for high throughput. Ensuring a secure and open environment requires disproportionate increases in equipment capabilities and efforts in the dynamic security policy configuration, event monitoring and analytics. We have started testing ethernet-port security in some networks, which also enables advanced features, such as autonomous registration of new devices, i.e., in computer lecture rooms and laboratories. A new cyber-security policy has been put in place for the reactor campus and we plan to use it as the basis for a new, Institute-wide security policy.

Internal development of e-mail security, dynamic network firewalling, encrypted connections, virtual networks, advanced analysis and monitoring ensure the security of an open academic network in the age of a hostile internet.
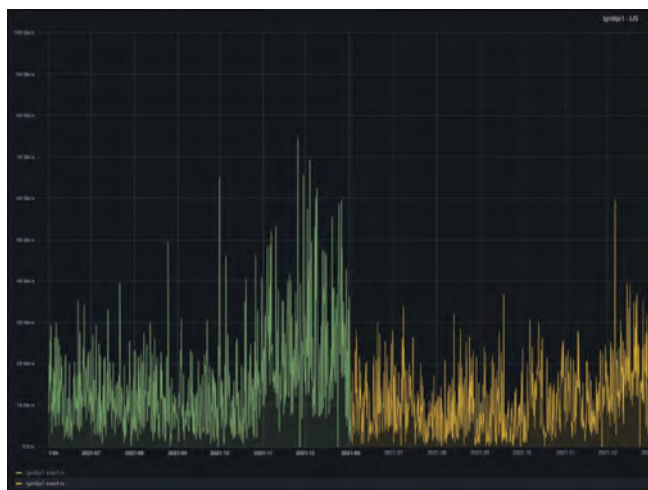

Figure 2: The new 100 Gbit/s connectivity shows high throughput at the JSI Computing Facility Teslova.

Since the NIC is responsible for the security of the ICT infrastructure of the Institute, we are active members of relevant institutions and groups, notably the national security response centre SI-CERT, FIRST (Forum of Incident Response and Security Teams) and EGI CSIRT (European Grid Initiative distributed computing security incident response team). We also take part in the response team of the national distributed computing network consortium SLING, where we also participate in the HPC Vega system's security team. The national science certificate agency SiGNET CA (Slovenian Grid Network Certification Authority), managed by the NIC, is a full member of EU Grid PMA (EU Grid Policy Management Authority) and IGTF (Interoperable Global Trust Federation). We participate in the work of Slovenian network technology and security association SINOG (Slovenian Network Operators Group).

E-Mail: In the area of e-mail security and protection against undesired or malignant messages we have continued to develop e-mail content filters and protective measures to continuously improve solutions and provide new and advanced features in e-mail message and protocol stack handling and filtering.

Cryptography and certification: We have continued with the integration of DNSSEC-signed internet domain names using automated mechanisms for the verification of the signatures and with gradual introduction of the DANE system (integration of TLS certificates with the DNS system) in e-mail transfers and publishing SSHFP records via DNS servers. The number of digital certificates used on the Institute's servers has continued to rise, mostly using free DigiCert server certificates, courtesy of Arnes and GÉANT. We have also continued expanding the use of TLS encryption by widely introducing "Let's Encrypt" certificates to many services. The number or users of our VPN infrastructure has been rapidly increasing. By expanding and updating the VPN infrastructure we ensured the availability of remote connectivity to support remote working during the Covid-19 pandemic.

ICT services. The NIC provisions, develops and maintains a number of core and several additional ICT services. The most important among these are e-mail (e-mail routing and delivery, in-box management, directory management, webmail services etc.) and world-wide-web support (main Institute web server, web hosting for users, departments and projects, a web directory). Secondary ICT services are provided in support of certain core or specific activities at the Institute, such as web presentations, a conference system, supervision and monitoring, etc. In some of these services the NIC is directly invested in the software or infrastructure development, such as the network time services and e-mail filtering and security, while others are simply administered and maintained. The third NIC service category is comprised of services supporting our users (calendaring, event management, directories, file sharing, collaborative editing) and software/system developers (code repositories, integration and verification, licence management, mobile platform software development, integration and shipping for Apple Appstore and Google Play). We also provide physical

Repositories for software development, file sharing and data storage as well as support for collaborative work and development have become essential for modern scientific collaborations. Large data storage and access to the best systems, including the new EuroHPC Vega and other new European HPC systems, have become a basic necessity for many researchers.

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 2021 we expanded the hosting in the computing centre at Teslova, established in 2015, to use the physical capacity to the limit of available electrical power at the location. The centre is now hosting the new Arnes HPC system, the most powerful HPC cluster in Slovenia at the time of installation, and has been used extensively for intensive computations.

The NIC computing centre at Jamova, where we can provide highly reliable cooling, network connectivity and an uninterrupted power supply for critical services, has accepted a number of new systems. Our web-hosting activity has expanded considerably (over 160 distinct sites) and started using new hardware.

We have continued the updating of our user-facing documentation and our user interfaces. A Single-Sign-On (SSO) service, integrated with the national AAI federation at Arnes and European eduGAIN federation is now used extensively since it gives our users easier access to numerous national and international services using their Institute credentials. We hope that this facility will simplify user and authentication management at the Institute and for software developers who work on internal projects and services in the future.
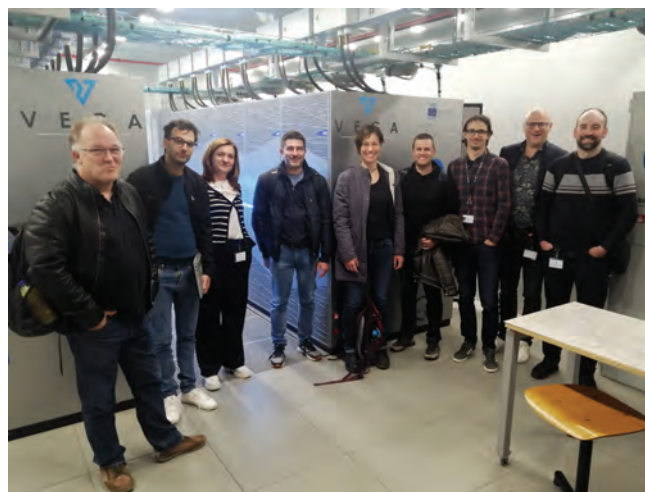
Network supercomputing. In the field of network supercomputing Slovenia decided to be the first country to set-up a HPC system in the new Europe-wide initiative EuroHCP. HPC Vega started operating in April and became the first system to accept European users through the initiative, setting new trends and attracting considerable attention. The Jožef Stefan Institute created a task force that profited from the long tradition and technical expertise at the NIC and the Experimental Particle Physics Department F9 that participated in the design, architecture, procurement, installation and operations of the new system that has been established at the IZUM data centre in Maribor. Within the Slovenian National Supercomputing Network SLING consortium we created a group that provided operational oversight, system administration support, user support, high-level support and guidance for the new system as Vega quickly became the most anticipated system in the EU, due to the high visibility of the EuroHPC initiative. Some of its technical innovations, such as large bandwidth and on-site storage, have been very successful and well accepted. We have also participated in the EUROCC project's training and support efforts with our expertise in high-throughput computing, high-performance computing, network and grid middleware, vectorisation, software containers, virtualisation and ICT as a service (cloud). The NIC also maintains the Slovenian certification agency SLING CA for science, research and grid computing, takes part in the maintenance and support of the core national supercomputing grid network services and coordinates work with international infrastructure projects and collaborations.

Figure 3: Located at IZUM, the new Slovenian supercomputer Vega was designed and set-up with support of JSI experts. The new system with close to 6.8 peta FLOP/s of raw computing power, 20 PB of storage and broadband connectivity has put Slovenia in 21st place in the November's Top500 list of supercomputing capacity per number of inhabitants.

In 2021 the New System Cluster (NSC) has fully utilised its last upgrade with AMD Epyc, NVidia Ampère 100 and Xilinx FPGA and almost 2 PB of distributed CEPH-based provided in collaboration with the E7 and E8 departments, Additionally, the new Arnes HPC system, hosted in the same location, which was the largest publicly available HPC cluster in Slovenia before Vega began operations, has seen extensive utilisation. Besides supporting users of JSI clusters, we also worked on the integration of clusters with the national supercomputing network SLING and Vega using the NorduGrid ARC Grid Middleware to enable users to use all the resources in the network with the same interfaces and to use software containers to facilitate the portability of user software.

In the domain of network supercomputing we have been most involved with the Slovenian National Supercomputing Network (SLING) and EuroHPC, but we also worked within the European Grid Initiative EGI, PRACE (Partnership for Advanced Computing in Europe), EuroHPC initiative, notably the EuroHPC Leonardo hosting entity consortium (operations expected in 2022), the NorduGrid ARC collaboration and a number of international projects (ATLAS – dedicated link, Belle2 – computing support, CLARIN – support for different services of Slovenian national node, ELIXIR – collaboration with the national node and the European collaboration). SLING has supported a number or research projects and applications, among others in high-energy physics, medical sensor and image analysis, theoretical physics, astrophysics, biochemistry, protein-folding simulations, crystal analysis, knowledge technologies, artificial intelligence, statistical analysis and fluid dynamics, computational linguistics, etc. In a number of cases we have been involved as part of the SLING support group in the parallelization and preparation of

HPC Vega is operated and maintained by a team of system engineers – including our own experts. Here in front of the location at IZUM in Maribor.

computing tasks and administration of the required run-time environments. Members of NIC have also contributed as advisers in the EuroHPC and European Open Science Cloud, HPC RIVR consortium expert committee, training and set-up of the new national supercomputer HPC RIVR Maister at the University of Maribor and the operational opening of Slovenian EuroHPC petascale site at IZUM with the HPC RIVER Vega machine.

INTERNATIONAL PROJECTS

1. EACEA: B-AIR; Art Infinity Radio - Creating Sound Art for Babies, Toddlers and Vulnerable Groups
   Dr. Jan Jona Javoršek
   Eacea - Education Audiovisual & Culture Executive Agency

2. H2020 - EUROCC; National Competence Centres in the Framework of EuroHPC
   Dr. Jan Jona Javoršek
   European Commission

3. H2020 - EGI-ACE; EGI Advanced Computing for EOSC
   Dr. Jan Jona Javoršek
   European Commission

STAFF

Technical officers
1. Jan Ivanjko, B. Sc.
2. **Dr. Jan Jona Javoršek, Head**
3. Barbara Krašovec, M. Sc.
4. Mark Martinec, B. Sc.

Technical and administrative staff
5. Ivan Ivanjko
6. Janez Jezeršek
7. Matjaž Levstek
8. Janez Srakar
9. Matej Wedam

SCIENCE INFORMATION CENTRE

SIC

The Jožef Stefan Institute Science Information Centre is one of the largest special libraries in Slovenia. We provide publication access, manage the Institute bibliography, and help our researchers to fulfil open-access mandate requirements.

The peer-reviewed publication of results in scientific journals is an important, basic part of the research process. Therefore, literature access is central to research quality and relevance. The information revolution and open-science movement have brought great changes to the publishing process, but access to most research is still restricted to subscribers. The article and journal inflation of recent years has focused our subscription policy on package deals with major publishers. We are a founding member of the ScienceDirect, SpringerLink, Wiley online library, IEEExplore, RSC and ACS Slovenian consortia, and negotiate with publishers to lower the reading and publishing costs for all Slovenian researchers. We provide access to over 4000 electronic journals. Our electronic collections are supplemented by over 100,000 print journal issues and books covering the fields of physics, chemistry, biochemistry, electronics, information science, artificial intelligence, nuclear technology, energy management and environmental science. We subscribe to the Reaxys database and the SciVal research-evaluation and management tool.

The Slovenian Current Research Information System, SICRIS, is the basis of all evaluation processes of the Slovenian Research Agency (ARRS). SICRIS data are stored in the COBISS database, which has records of the Institute's research since its founding in 1949. We manage the bibliographic data for approximately 700 researchers in the COBISS database, and provide evaluation reports used in the election process at the Institute. Last year's bibliographic data are included as part of this report.

Open-access mandates have become a common part of the research environment. Slovenia adopted an open-access strategy, ARRS is a Plan S member, and requires compliance with its mandates. Preprint publication in a repository is a part of these requirements. We help researchers to comply by depositing their work in the DIRROS repository, which is OpenAire compatible.

Head:
Dr. Luka Šušteršič

STAFF

Technical officers
1. **Dr. Luka Šušteršič, Head**
2. Marjan Verč, M. Sc.

Technical and administrative staff
3. Suzi Korošec, B. Sc.
4. Jasna Malalan

5. Katarina Modic, B. Sc.
6. Alenka Ana Stante, B. Sc.
7. Jože Škulj
8. Branka Štrancar
9. *Ana Tratnik, B. Sc., left 01.08.21*
10. Saša Žnidar, B. Sc.

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1. Marijan Ribarič, Luka Šušteršič, "On simplified models for dynamics of pointlike objects", *Journal of applied mathematics and physics*, 2021, **9**, 8, 1853-1869.

ENERGY EFFICIENCY CENTRE
EEC

The basic activities of the Energy Efficiency Centre are in efficient energy use, long-term planning in energy and the reduction of greenhouse-gas (GHG) emissions and other air pollutants. 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, GHG emissions and air pollutants. Nevertheless, it still remains strongly connected, by its consulting and training role in energy, with industrial companies and other institutions as well as also being deeply involved in European research projects.

Head:
Stane Merše, M. Sc.

Energy and the Environment

In 2021 the EEC with its professional work ensured high-quality support to ministries in the preparation of the strategic development documents and transfer of EU legislation. Energy efficiency is a priority field to achieve global climate and energy goals and in accordance with the Directive on Energy Efficiency (2012/27/EU) EEC report on the implementation of the Action plan for 2019. With the approval of the government, the preparation of the Long-Term Renovation Strategy of Buildings until 2050 was completed, and we began the preparation of the analytical basis for the development of measures for energy-poverty mitigation.

Within the expert support of the Ministry of Environment and Spatial Planning, the EEC activities focused on the preparation of a draft Long-Term Climate Strategy for Slovenia to 2050, which ended with the adoption of a resolution in the National Assembly in July 2021. It was based on the analytical basis and long-term GHG emission projection within the LIFE ClimatPath2050 project with a goal to contribute to better climate governance by enhanced monitoring and planning of GHG-mitigation measures in buildings, transport, industry, agriculture, forestry and waste and was successfully completed at the end of 2021. The fourth Climate Action Mirror was prepared, which also presents a report on the implementation of the Operative Programme of Measures for GHG-emission reduction until 2020 and the Local Climate Activity Scoreboard of Municipalities. The EEC continued with activities of the LIFE IP CARE4CLIMATE - Boosting greenhouse-gas emissions reduction by 2020 with a view to 2030, where the EEC leads several actions on training, local energy planning and the development of advanced instruments for sustainable buildings' retrofit. The EEC was also involved in the preparation of an analytical basis for international reporting in the framework of the MMR, started with the preparation of analytical bases for fulfilling national, European and international reporting obligations. The EEC continued its preparation of the professional support for the design of National Air Pollution Control Programmes (NAPCP).

The EEC cooperates with the Statistical Office of the Republic of Slovenia, where it annually prepares a model calculation for fuels and energy use in households for the national energy statistics; however, it began with a study of energy use in the service sector and an analysis of the utilization of excess heat. Also in 2020, the EEC continued with activities of the state referential centre for energy with the preparation of an expanded set of indicators for energy and the environment. For the Energy Agency the

Figure 1: Final LIFE Climatepath2050 project results and impacts.

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, the exploitation of renewables and the transition of Slovenia to a carbon-neutral society, with training activities and support to industry it contributes to an increase in competitiveness and a successful green-technology transition.

Figure 2: New training programme in the field of energy management in the public sector (LIFE IP CARE4CLIMATE).
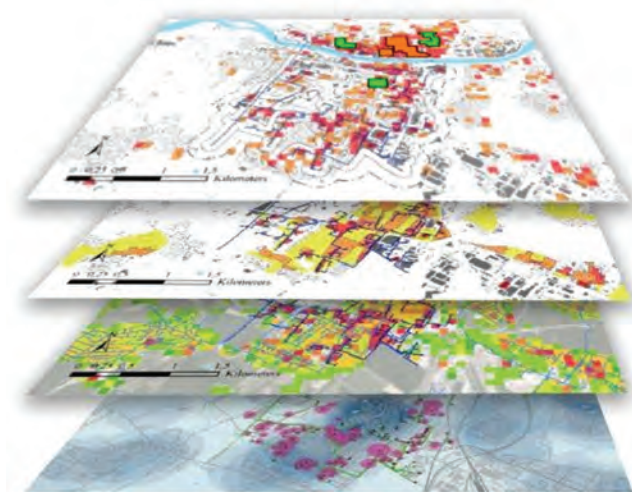

Figure 3: Methodological approach to the identification of "areas of opportunity" (areas marked on the map at the very top) by considering the geospatial characteristics of energy use and supply, RES potentials, infrastructure, development plans, constraints and other factors that influence the planning and implementation of local energy concepts.

Figure 4: Tools and services design for successfully creating energy communities within the CREATORS project.

EEC set new reference electricity generation costs for 2021 for the support scheme for RES and cogeneration electricity generation.

Promotion of Efficient Energy Use and Energy Consulting

In 2021 the EEC continued with its training activities where, as part of the LIFE IP CARE4CLIMATE project, a new comprehensive training programme was launched in the field of energy management in industry and the public sector, as well as energy contracting. The EEC continued with the thirteenth cycle of energy managers training within the European programme EUREM. Due to a very positive reaction of the participants and their interest (in Slovenia there is already more than 240 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.

In 2021 the EEC continued its intensive development work in the field of local energy planning with the further development of the GIS tool for the spatial analysis of heat consumption in buildings ("heatmap"). The GIS tool was used for the preparation of the Comprehensive assessment of the potential for efficient heating and cooling in Slovenia, a National heating and cooling strategy and upgrading the methodology for the preparation of local energy concepts.

The EEC continued its environmental assessments of the projects financed by green bounds in 2019 for SID bank and began with a calculation of the carbon footprint for the NLB Group. Successful development occurred for the Strategy of energy and resource efficiency and renewable energy sources for the sustainable development of the company DARS d. d. until 2030 and completed energy audits of AMZS and URI Soča buildings. EEC continued cooperation with the company SIJ Metal Ravne in the field of waste-heat utilisation.

The EEC prepared the programme for the 23rd conference "Energy Managers Days", the annual meeting of energy managers with more than 200 participants confirms the quality and public profile of the EEC's professional work.

International Cooperation

In 2021 the EEC carried out as many as 12 international projects, financed from the European Union's resources in the framework of LIFE, HORIZON 2020, ERASMUS+ and EUKI programmes. The projects cover activities in the fields of:

- Slovenian mid-century climate path (LIFE ClimatePath2050),
- Boosting greenhouse-gas emissions reduction by 2020 with a view to 2030, (LIFE IP CARE4CLIMATE),
- Heat-pipe technology for the waste heat recovery in industry (ETEKINA),
- Monitoring of indicators of for energy use and energy efficiency in the EU – (ODYSSEE MURE),
- Making heating and cooling for European consumers efficient, economically resilient, clean and climate-friendly(REPLACE),
- Creating Community Energy Systems – (CREATORS),
- Towards Innovative Methods for Energy Performance Assessment and Certification of Buildings (TIMEPAC),
- Streamlining Energy-Savings Calculations – (streamSAVE),
- Mainstreaming of Refinancing Schemes as Enhancer for the implementation of energy-efficiency projects - (REFINE),
- EU climate dialog – (EUKI, Climate Recon 2050),
- Energy-Efficiency Experts, (EEE, ERASMUS+),
- Carrying out the EU directive on energy efficiency (CA – EED2).

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 the EEC staff took part in numerous foreign professional meetings and visits.

Some outstanding achievements in the past three years

1. **Preparation of several key support documents for the government of the Republic of Slovenia** in the field of energy and climate policy: National Energy and Climate Plan - NECP), Long-term climate strategy for Slovenia until 2050, Long-term renovation strategy to support the renovation of national building stock into a highly energy efficient and decarbonised building stock by 2050, etc. and establishment of a comprehensive monitoring system, implementation of the climate and energy policy (Climate Mirror, ARSO environmental indicators, etc.)

2. **Establishment of energy-managers training** in the framework of the European project EUREM and new comprehensive training programme for the transition to a low-carbon society of the LIFE IP CARE-4CLIMATE project.

3. **Professional support to industry and other institutions** for successful green technology transition: Strategy of energy and resource efficiency and renewable energy sources for the sustainable development of the company DARS d. d. until 2030, by carrying out energy audits and other consulting (Luka Koper, Ljubljanske mlekarne, BTC, AMZS etc.). Preparation of the **European code of Conduct for energy contracting** and design of new financial instruments with ECO Fund.

Organization of conferences, congresses and meetings

1. EUREM educating, RCP, Brinje, January–December 2021 (due to COVID-19 only partially implemented in 2020, with the rest in 2021)

2. Workshop on the LIFE Climate Path 2050 Project: Presentation of the background analysis for the strategy regarding the agriculture and LULUCF sectors, 3 March, 2021, virtual

3. LIFE Climate Path 2050 Workshop: Presentation of background analysis for Slovenian Long-term climate strategy until 2050 (with presentation of models) – for JSI, 2 April, 2021, virtual

4. LIFE Climate Path 2050 Workshop: Presentation of the Analysis of GHG Emission Reduction Scenarios for Transport until 2050, 15 April, 2021, virtual

5. Workshop on the LIFE Climate Path 2050 Project: Presentation of the background analysis for the strategy in Slovenia until 2050, 17 April, 2021, virtual

6. Training course for energy contracting for state and municipal officers and enterprises, LIFE IP Care4Climate, 20 – 22 April, 2021, virtual

7. Consultation on the LIFE Climate Path 2050 Project: Tools Supporting Planning in Local Communities, 23 April, 2021, virtual

8. LIFE Climate Path 2050 Workshop: Presentation of the background analysis for the Long-term Climate Strategy up to 2050 of Slovenia, 26 May, 2021, virtual

9. Training course for energy management in the public sector, LIFE IP Care4Climate, 8–10 June 2021, virtual

10. Workshop of the LIFE Climate Path 2050 Project: Presentation of expert bases for Slovenia's Long-Term Climate Strategy until 2050 for the general public, 9 June, 2021, hybrid event: JSI, Brinje and virtual

11. Training course for energy management in the industry, LIFE IP Care4Climate, 15–17 June, 2021, virtual

12. Coordination of the Main Recommendations and Highlights of the Climate Action Mirror 2021, online event, 14 September, 2021, virtual

13. Consultation on the LIFE Climate Path 2050 Project: Workshop on models and methods for GHG emission projections up to 2050, 15 September, 2021, hybrid event: Faculty of Social Sciences and virtual

14. 23rd Energy Managers Conference – When, if not now? Energy efficiency on a wave of green recovery, 20-21 September, 2021, Portorož, co-organising

15. LIFE CLimatePath2050 International Conference: Designing pathways towards Climate Neutrality, 6-8 October, 2021, hybrid event: The Slovenian Forestry Institute and virtual

16. LIFE Climate Path 2050 Project Workshop: Traffic projections in Slovenia until 2050, 20 October 2021, hybrid event: JSI, Brinje and virtual

17. LIFE Climate Path 2050 Presentation of solar energy rooftop potential in Slovenia - roofs orientation analysis, 17. November, 2021, virtual

18. Energy and material efficiency strategy of DARS, d.d. until 2030, presentation for the management of DARS, 17 November, 2021, virtual

19. Consultation on the LIFE Climate Path 2050 Project: How to get to good climate governance and climate act? Seminar on climate governance in Slovenia, 18 November, 2021, virtual

20. Training course for energy renovation of buildings for energy managers in the public sector and industry, designers, heads of maintenance and energy, LIFE IP Care4Climate, 23 – 25 November, 2021, virtual
21. Joint H2020 project ODYSSEE-MURE and LIFE Climate Path 2050 Workshop: energy efficiency first, 29.11.2021, virtual
22. Consultation on the LIFE Climate Path 2050 Project: How to get to good climate governance and climate act? Seminar on climate act in Slovenia, 30 November, 2021, virtual
23. Consultation on the LIFE Climate Path 2050 Project: Seminar on analytical background on energy poverty, 2 December, 2021, virtual
24. Consultation on the LIFE Climate Path 2050 Project: How to get to good climate governance and climate act? - Final seminar, 8 December, 2021, virtual
25. Consultation on the LIFE Climate Path 2050 Project: Seminar on challenges and strategic direction in the heating and cooling sector, 10 December, 2021, virtual
26. TIMEPAC workshop on innovative methods and approaches for energy efficiency assessment and energy performance certification of buildings, 14 December, 2021, virtual

INTERNATIONAL PROJECTS

1. Life IP Care4Climate - Boosting greenhouse gas emissions reduction by 2020 with a view to 2030
2. Stane Merše, M. Sc.
   European Commission
3. European Climate Initative (EUKI) - EU Climate Action Dialogues
   Katarina Trstenjak
   Europäische Klimaschutzinitiative (euki)
4. ERASMUS+; EEE - Energy Efficiency Expert
   Dr. Boris Sučić
   Inapp - Istituto Nazionale Per L'analisi
5. „LIFE ClimatePath 2050" Slovenian Path towards the Mid-Century Climate Target
   Andreja Urbančič, M. Sc.
   European Commission
6. H2020 - ETEKINA; Heat Pipe Technology for Thermal Energy Recovery in Industrial Applications
   Dr. Fouad Al-Mansour
   European Commission
7. H2020 - ODYSEE-MURE; Monitoring EU Energy Efficiency First Principle and Policy Implementation
   Dr. Fouad Al-Mansour
   European Commission
8. H2020 - REPLACE; Making Heating and Cooling for European Consumers Efficient, Economically Resilient, Clean and Climate-Friendly
   Dr. Gašper Stegnar
   European Commission
9. H2020 - REFINE; Mainstreaming of Refinancing Schemes as Enhancer for the Implementation of Energy Efficiency Service Projects
   Damir Staničić, M. Sc.
   European Commission
10. H2020 - streamSAVE; Streamlining Energy Savings Calculation
    Dr. Matevž Pušnik
    European Commission
11. H2020 - CREATORS; Creating Community Energy Systems
    Dr. Boris Sučić
    European Commission
12. H2020 - TIMEPAC; Towards Innovative Methods for Energy Performance Assessment and Certification of Buildings
    Dr. Boris Sučić
    European Commission

RESEARCH PROGRAMME

1. Modelling and environmental impact assessment of processes and energy technologies
   Dr. Fouad Al-Mansour

R&D GRANTS AND CONTRACTS

1. Eco innovation and circular economy - a path toward a more sustainable and inclusive future: the role of demographic changes and digitalization
   Dr. Boris Sučić
2. Investigation of turbulent heat transfer in an annulus through advanced experimental and computational methods
   Asst. Prof. Marko Matkovič
3. Preparation of expert documents, design of a database and development of a vehicle simulation model for calculation of the energy and environmental footprint with an aim to optimize implementation of the public transport service
   Dr. Marko Kovač
4. Preparation of strategic studies for elaboration of strategic documents, action plans and measures from the field of energy
   Stane Merše, M. Sc.
   Ministry of Infrastructure
5. Concerted actions in the field of the directive on renewable energy (CA RES)
   Stane Merše, M. Sc.
   Ministry of Infrastructure
6. Concerted Action 2 – Energy Efficiency Directive: National experts participation
   Stane Merše, M. Sc.
   Ministry of Infrastructure
7. Cofinancing of LIFE ClimatePath 2050: Slovenian Path towards the Mid-Century Climate Target
   Andreja Urbančič, M. Sc.
   Ministry of the Environment and Spatial Planning
8. National Air Pollution Control Programme (OP-NEC)
   Matjaž Česen, B. Sc.
   Ministry of the Environment and Spatial Planning
9. Cofinancing of the Project LIFE17 IPC7SI/000007 - LIFE IP CARE4CLIMATE
   Stane Merše, M. Sc.
   Ministry of the Environment and Spatial Planning
10. Preparation of draft of Long term climate strategy of Slovenia 2050 and support with the coordination of the document
    Katarina Trstenjak
    Ministry of the Environment and Spatial Planning

NEW CONTRACTS

1. Environmental impact assessment
   Stane Merše, M. Sc.
   SID banka, d. d., Ljubljana
2. Participation in the implementation of the energy audit for 25 selected AMZS facilities
   Luka Tavčar, B. Sc.
   AMZS d. d.

VISITOR FROM ABROAD

1. Prof. Hussama Jouhara, Brunel University, London, Great Britain, August 12, 2021, one-day visit

STAFF

Researchers
1. Dr. Fouad Al-Mansour
2. Asst. Prof. Marko Matkovič
3. **Stane Merše, M. Sc., Head**
4. Damir Staničić, M. Sc.
5. Andreja Urbančič, M. Sc.

Postdoctoral associate
6. Dr. Matevž Pušnik

Technical officers
7. Matjaž Česen, B. Sc.
8. Jure Čižman, M. Sc.
9. Tomaž Fatur, M. Sc.
10. Edvard Košnjek, M. Sc.

11. Dr. Marko Kovač
12. Marko Pečkaj, B. Sc.
13. Barbara Petelin Visočnik, M. Sc.
14. Dr. Gašper Stegnar
15. Dr. Boris Sučić
16. Luka Tavčar, B. Sc.

Technical and administrative staff
17. Marko Đorić, B. Sc.
18. Tadeja Janša, B. Sc.
19. Marija Kavčič, B. Sc.
20. Igor Ribič
21. Katarina Trstenjak, B. Sc.

BIBLIOGRAPHY

ORIGINAL ARTICLE

1. Boštjan Zajec, Marko Matkovič, Nejc Kosanič, Jure Oder, Blaž Mikuž, Jan Kren, Iztok Tiselj, "Turbulent flow over confined backward-facing step: PIV vs. DNS", *Applied sciences*, 2021, **11**, 22, 10582.
2. Boris Sučić, Stane Merše, Marko Kovač, Zeljko Tomsic, "Challenges of combining different methods and tools to improve the performance monitoring in buildings: A case study of elementary schools and kindergartens", *Energy and buildings*, 2021, **231**, 110608.

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1. Barbara Petelin-Visočnik, Andreja Urbančič, Matjaž Česen, Tadeja Janša, "Monitoring climate and energy policy implementation - how to take a step forward", In: *ECEEE 2021 Summer Study on energy efficiency: a new reality?, 7-11 June 2021*, Proceedings, European council for an energy efficient economy, 2021, 4-127.
2. Ivan Todorović, Ivana Isakov, Boris Sučić, Aleksandar Kavgić, Dušan Čohadžić, "Advances in distributed generation source digital twins design", In: *SP2021, 9th edition of Sustainable Places, 29 September–1 October 2021, Rome, Italy*, Proceedings (Environmental sciences proceedings **11**), 2021, 1, 2.
3. Fouad Al-Mansour, Matevž Pušnik, Kristijan Plesnik, Marko Pečkaj, Stane Merše, Marko Matkovič, "Heat pipe heat exchanger system for the utilization of excess heat in the steel industry", In: *WECC 2021, International conference on water, energy & climate change, 25-28 October 2021, Sharjah, United Arab Emirates*, University of Sharjah, 2021.
4. Jure Čižman, Stane Merše, "Prenove sistemov daljinskega ogrevanja – ovire, priložnosti in podporni ukrepi", In: *Energy supply and use in smart buildings and homes, Portorož, 28-29 June 2021*, zbornik prispevkov, Slovensko združenje za energetiko, 2021.
5. Damir Staničić, Jure Čižman, Marko Matkovič, Stane Merše, Joerg Prestor, Janja Svetina, Miran Rožman, Ljubo Germič, "Raba hidrotermalne in plitve geotermalne energije v sistemu daljinskega ogrevanja mesta Maribor", In: *Energy supply and use in smart buildings and homes, Portorož, 28-29 June 2021*, zbornik prispevkov, Slovensko združenje za energetiko, 2021.
6. Edvard Košnjek, Boris Sučić, Marko Kovač, Stane Merše, "Energetske skupnosti kot instrument pravičnega prehoda in razvoja trajnostne infrastrukture - nov postopek ocenjevanja potencialov OVE v povezavi z dejansko rabo energije", In: *15. konferenca slovenskih elektroenergetikov CIGRE-CIRED, Thermana Laško, 19-21 October 2021*, Referati in predstavitve, Slovensko združenje elektroenergetikov CIGRE-CIRED, 2021, C1-112.
7. Boris Sučić, Edvard Košnjek, Matevž Pušnik, Jure Čižman, Stane Merše, Franc Cimerman, Anton Munih, Andrej Stušek, Tomaž Vuk, "Energetske skupnosti kot platforma za doseganje ciljev trajnostnega razvoja in povezovanje energetsko intenzivne industrije, energetskih omrežij in lokalnega prebivalstva", In: *15. konferenca slovenskih elektroenergetikov CIGRE-CIRED, Thermana Laško, 19-21 October 2021*, Referati in predstavitve, Slovensko združenje elektroenergetikov CIGRE-CIRED, 2021, C1-146.

INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Danijel Crnčec, Boris Sučić, Stane Merše, "Slovenia: drivers and challenges of energy transition to climate neutrality", In: *From economic to energy transition*, (Energy, Climate and the Environment), Palgrave Macmillan, 2021, 247-282.

SCIENTIFIC MONOGRAPH

1. Marko Kovač, *Energetske potrebe človeštva skozi čas: od industrijske revolucije do civilizacije tipa I*, Založba ZRC, 2021.

PROFESSIONAL MONOGRAPH

1. Barbara Petelin-Visočnik, Andreja Urbančič, Katarina Trstenjak, Gašper Stegnar, *Climate path towards the mid-century climate target: LIFE ClimatePath2050*, LIFE, 2021.

CENTRE FOR ELECTRON MICROSCOPY AND MICROANALYSIS CEMM

The Centre for Electron Microscopy and Microanalysis (CEMM) is an instrumental centre at the JSI that comprises analytical equipment for electron microscopy and microanalysis. Access to the research equipment within the CEMM is available to the JSI departments as well as other research institutions, universities and industrial partners. The equipment in the CEMM is used by researchers interested in the morphology and structural or chemical characterization of materials at the micrometre and atomic level. The CEMM comprises four scanning electron microscopes (JSM-7600F, Verios G4 HP, Quanta 650, JSM-5800), two transmission electron microscopes (JEM-2100 (CO NiN) and JEM-2010F) and the equipment for TEM and SEM sample preparation. Additionally, the IJS is a co-owner (20 %) of a JEM-ARM200CF at the Chemical Institute.

Head:
Prof. Miran Čeh

High-resolution scanning electron microscope Verios G4 HP, Thermo Fisher Scientific, (Figure 3) is unique in this part of Europe and provides extremely high imaging resolution at low accelerating voltages. It also features automatic sample insertion and the ability to observe non-conductive specimens with exceptional Z-contrast, even at low voltages. In addition to a highly sensitive EDXS detector, the microscope is equipped with a transmission detector (STEM) as well.

Scanning electron microscope Quanta 650, Thermo Fisher Scientific, (Figure 4) operates in three vacuum ranges that are achieved through differential pumping. This allows us to investigate a wide range of materials, both conductive and non-conductive.

The research carried out using the equipment in the CEMM is diverse due to many different research topics of the JSI departments:

– Scanning electron microscopy is employed to observe the morphology and structure of surfaces and for the microstructural investigation and determination of the chemical composition of the investigated materials. Samples that are most frequently investigated are ceramics (polycrystalline oxide and non-oxide compositions), nanostructured materials, metallic magnetic materials, metals, alloy glass, etc. All of the scanning electron microscopes in the CEMM are equipped with an energy-dispersion (EDXS) and/or wavelength-dispersion (WDXS) spectrometer for X-rays, allowing non-destructive determination of the chemical composition of the investigated materials. The JSM-7600F scanning electron microscope is additionally equipped with an electron back-scattered diffraction (EBSD) detector and an electron lithography system. The Verios 4G HP microscope enables the observation of the morphology of nanoparticles and samples that are sensitive to electron doses. The Quanta 650 microscope allows the observation of larger conductive or non-conductive samples.

Figure 1: Centre for Electron Microscopy and Microanalysis (CEMM)

– Transmission electron microscopy (TEM) provides an insight into the structure of a material on the nano-scale (the atomic level). Transmission electron microscopy enables structural and chemical analyses of nanostructured phenomena, such as grain boundaries, precipitates, planar defect, dislocations, etc. Materials that are investigated include thin films on different substrates, alloys, metallic magnetic materials, dielectric materials, ferroelectrics, etc. The JEM-2100 transmission electron microscope is equipped with an EDXS spectrometer and a CCD camera, while the JEM-2010F is additionally equipped with a scanning transmission electron (STEM) unit, EDXS and EELS (electron energy loss) spectrometers and a CCD camera. The ARM200CF is a dedicated scanning transmission electron microscope with ADF, HAADF, ABF STEM detectors and GIF system.

– The CEMM also manages the necessary equipment for the SEM and TEM sample preparation.

Figure 2: JSM-7600F scanning electron microscope

The operation of the Centre is managed by the CEMM personnel. Besides the maintenance of the equipment, other CEMM activities include, among others, training of new operators, organization of workshops and conferences on the topic of electron microscopy, providing services for industrial partners and implementation of new analytical techniques. The CEMM personnel are also
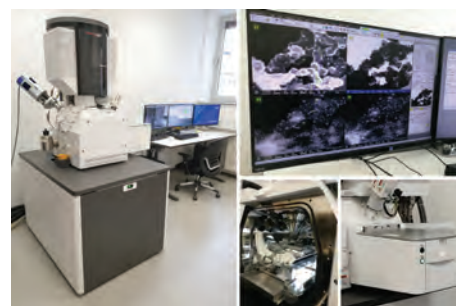

Figure 3: Verios 4G HP scanning electron microscope

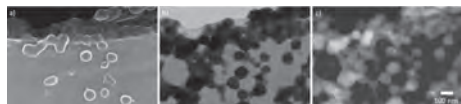*Figure 4: ESEM Quanta 650 scanning electron microscope*

Figure 5: Dissolved active substance images: a) SEM mode, b) STEM bright field mode, c) STEM HAADF mode (Jitka Hreščak, CEMM, SEM Verios G4 HP)
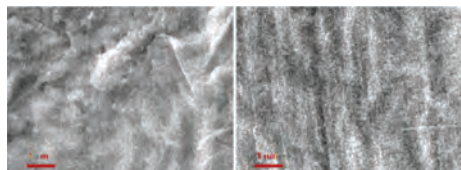

Figure 6: SEM images of the sliding surface of a cross-country ski before (left) and after (right) the ski surface was waxed with a wax for dry snow (Polona Umek, IJS-F5, Miha Plesnik)
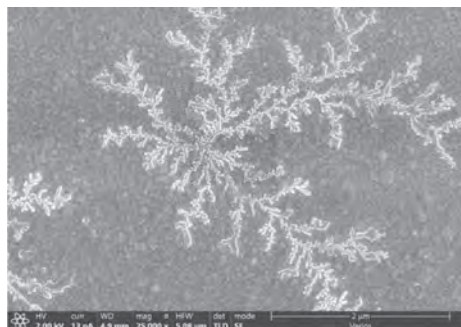

Figure 7: SE SEM image of a 'silane snowflake' (Darja Lisjak, K8)
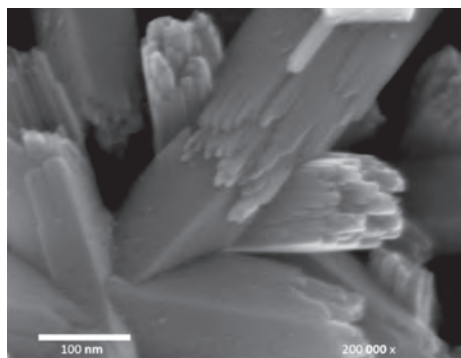

Figure 8: SEM image of rutile nanorods (Zoran Samardžija, K7, Verios G4 HP)

responsible for the dissemination of electron microscopy techniques to the general public in the scope of organized visits to the IJS, as well as through publications in traditional and digital media.

Examples of microstructural and nanostructural investigations of materials performed with the CEMM equipment

Below are examples of analyses of structural and chemical characterisations of different materials performed by the operators from different JSI departments and the CEMM personnel, using electron microscopy techniques.

1. Dissolved active pharmaceutical substance

An analysis of a dissolved pharmaceutical active substance was performed in the Verios 4G HP scanning electron microscope in the SEM mode, STEM bright field mode and STEM HAADF mode (Figure 5).

2. Sliding surface of a cross-country ski

Polymer coatings for skis were analysed in a scanning electron microscope before and after wax coating. The work was done in collaboration with the Faculty of Polymer Technology in Slovenj Gradec and the Ski Association of Slovenia (Figure 6).

Ref.: M. Plesnik, diploma thesis, 2021, 56 pages

3. Silane snowflake

A SEM micrograph of silane polycondensation on a glass substrate is shown in Figure 7.

4. Rutile nanorods

A high-resolution SE micrograph of the termination of rutile nanorods is shown in Figure 8. The image was recorded with the Verios 4G HP scanning electron microscope at a 200,000× magnification.

5. Characterization of a nanocomposite based on graphene and polypyrrole nanoballs

Morphological features of PPy@Graphene were observed using a high-resolution transmission electron microscope (HRTEM) (JEM 2100, JEOL Ltd.) and an AG-Ultra 55 (Zeiss) field-emission scanning electron microscope (FESEM) (Figure 9).

Ref.: J. Casanova-Chafer, P. Umek, S. Acosta, C. Bittencourt, E. Llobet, ACS Applied Materials & Interfaces, ISSN 1944-8244, 2021, 13, 34, 40909–40921.

6. Morphological characterization of the WS₂ nanostructure

The microstructure of WS_2 was characterized using a SEM-FEI Quanta 600 scanning electron microscope. High-resolution transmission electron microscopy (HRTEM) was used to analyse the crystal structure at the atomic level (Figure 10).

Ref.: A. Alagh, F. E. Annanouch, P. Umek, C. Bittencourt, A, Sierra-Castillo, E. Haye, J. F. Colomer, E. Llober, Sensors and Actuators B: Chemical, 2021, 326, 128813-1-128813-11.

7. Ferroelectric domains in ceramics

A SEM analysis of ferroelectric domains in the $Pb(Mg_{1/3}Nb_{2/3})O_3$-0.4PbTiO$_3$ ceramic in the virgin state and after an ex-situ application of an electric field of ~10 kV/cm is shown in Figure 11.

Ref.: M. Otoničar et al., Open Ceramics, 2021, 7, 100140.

8. EDS analysis of the Ti/V layer in a multilayer ceramic component

EDS mapping was used to detect Ti/V layers within a multilayer ceramic component (Figure 12).

9. STEM analysis of an LSCO/(100)LSGM thin film

High-angle annular dark-field (HAADF) STEM and annular bright-field (ABF) of an LSCO/(100)LSGM thin film deposited with the PLD technique showed an order-free zone between the LSCO and LSGM layers (Figure 13).
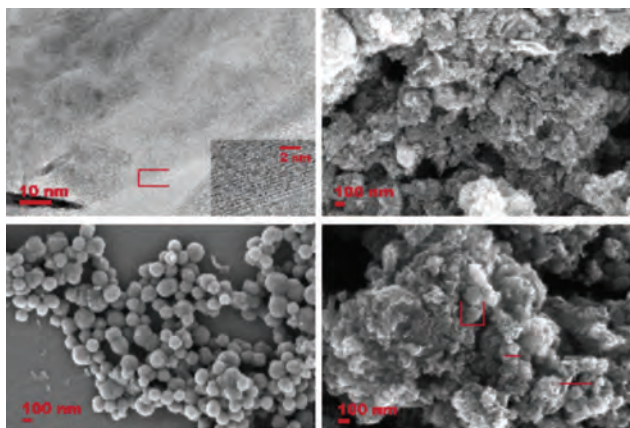
Figure 9: Top: TEM and SEM images of bare graphene. The inset in the TEM image shows the layered graphene structure (the red frame in the image indicates the area of the inset). Bottom left: SEM images of synthesized polypyrrole nanoparticles (PPy NPs). Bottom right: graphene nanoflakes decorated with PPy NPs. Red squares help spotting the PPy NPs on loaded graphene (Polona Umek, JSI-F5, AG-Ultra 55, JEM-2100)
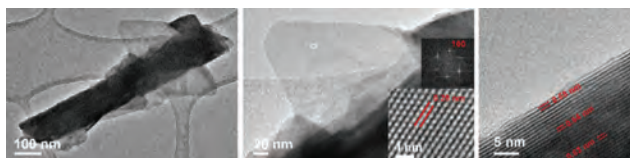
Figure 10: Left: TEM image of a WS_2 nanoneedle with a diameter of 125 nm and length of 800 nm. Middle: a triangular WS_2 nanosheet growing from the nanoneedle's longest side. The white frame in the image indicates the area where the HRTEM image was taken (the bottom inset); the upper insert is the corresponding FFT pattern. Right: HRTEM images of a side wall of the WS_2 nanoneedle (Polona Umek, JSI-F5, Quanta 600, JEM-2100)
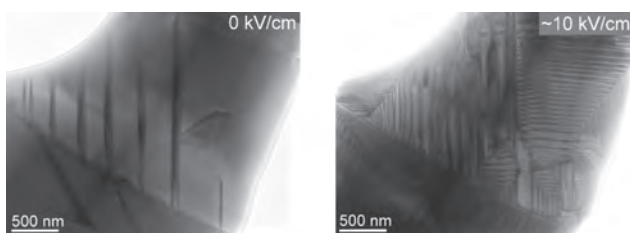
Figure 11: SEM image of ferroelectric domains in $Pb(Mg_{1/3}Nb_{2/3})O_3$-$0.4PbTiO_3$ ceramic in the virgin state (left) and after an ex-situ application of an electric field of ~10 kV/cm (right) (Mojca Otoničar, K5)
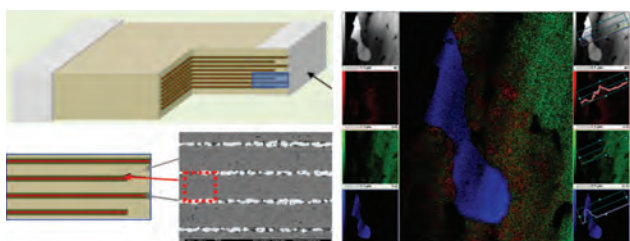
Figure 12: EDS mapping of the multilayer (Sandra Drev, CEMM, JEM-ARM200F)

Figure 13: HAADF STEM and ABF STEM images of the free zone in the LSCO/(100)LSGM thin film (Sandra Drev, CEMM, JEM-ARM200F)
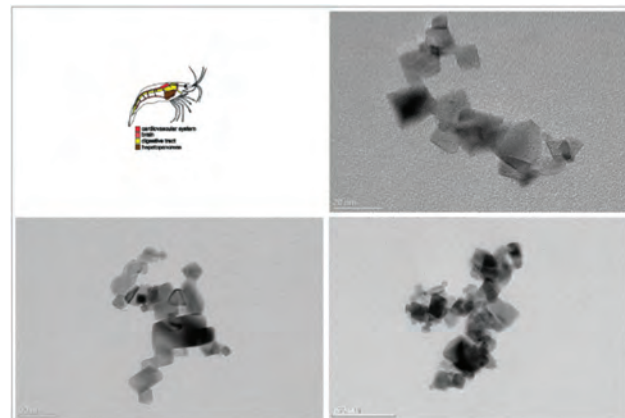
Figure 14: TEM images of CeO_2 NPs. Top left: pristine CeO_2 NPs, top right: [Ce-141]CeO_2 and bottom: [Ce-139/Ce-141]CeO_2 NPs (Sandra Drev, CEMM, JEM-2100)
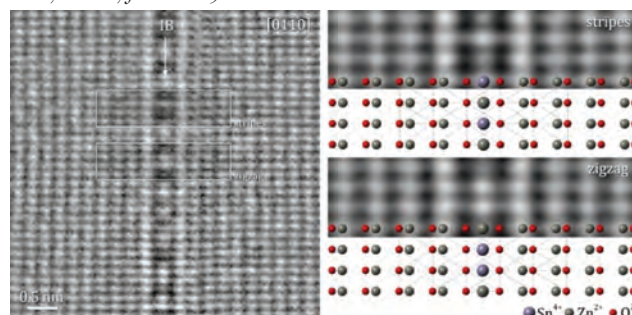
Figure 15: Quantitative HRTEM study of the Sn-rich IB in the [0110] projection: (a) Highresolution HRTEM image with an evident cation distribution along the IB-plane. Two typical sequences are observed (outlined). The simulated HRTEM images are based on (b) zigzag and (c) stripe cation ordering with overlaid structure models. Simulated images were calculated for a 2.8 nm thick crystal and a focus value of 72 nm. (Tina Radošević, F7/F9, Vesna Ribić)
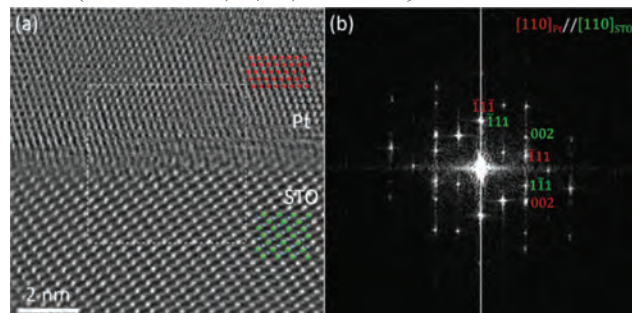
Figure 16: HAADF-STEM image of the Pt/STO interfacial region with the superimposed structural models viewed along the [110]Pt and [110] STO zone axes. Pt, Sr and Ti atoms are red, green and blue. (b) The corresponding FFT pattern is obtained from the marked area (a) (Sorour Semsari Parapari, K7)
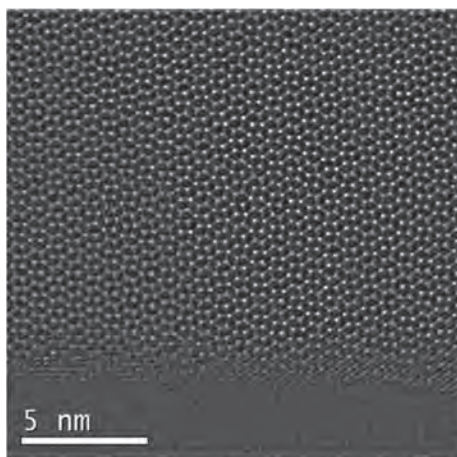
Figure 17: Atomically-resolved HAADF-STEM image of $Al_{13}Co_4$ intermetallic alloy (Sorour Semsari Parapari, K7)
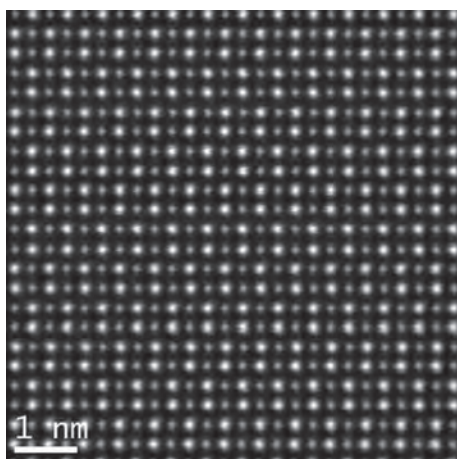
Figure 18: Atomically-resolved HAADF-STEM image of a wulfenite ($PbMoO_4$) crystal. Pb and Mo atoms are visible as bigger and smaller dots, respectively (Sorour Semsari Parapari, K7)

10. CeO_2 nanoparticle dissolution

A TEM analysis of CeO_2 nanoparticles taken from a freshwater shrimp was performed to study the differences between the radio-labelled nanoparticles from the original batch and the original nanoparticles (Figure 14).

Ref.: S. Schymura, I. Rydkin, S. Uygan, S. Drev, R. Podlipec, T. Rijavec, A. Mansel, A. Lapanje, K. Franke, M. Strok, Environmental Science: Nano, 2021, 8, 1934.

11. Study of the Sn-rich inversion boundary in ZnO

A quantitative HRTEM study of the Sn-rich inversion boundary in ZnO showed two different short-range arrangements of cations in the IB-plane. Cation arrangements (stripes and zigzag) are controlled by the IB chemistry and 6-fold in-plane symmetry limitations (Figure 15).

Ref: Ribić et al., Acta Materialia, 2021, 53, 237–252.

12. TEM study of Pt/STO

A TEM study of the position of a Pt/STO interfacial region with the superimposed structural models viewed along the $[110]_{Pt}$ and $[110]_{STO}$ zone axes was carried out (Figure 16).

13. TEM study of the $Al_{13}Co_4$ intermetallic alloy

An atomically-resolved HAADF-STEM image of the $Al_{13}Co_4$ intermetallic shows the atom positions within the structure (Figure 17).

14. TEM study of a wulfenite ($PbMoO_4$) crystal

An atomically-resolved HAADF-STEM image of a wulfenite ($PbMoO_4$) crystal shows the arrangement of atoms in a unit cell. Heavier Pb atoms are resolved as brighter dots (Figure 18).

INTERNATIONAL PROJECTS

1. Investigation of Helium Retention in Plasma Facing Materials Using Advanced Analytical Methods
   Andreja Šestan Zavašnik, B. Sc.
   Slovenian Research Agency
2. HE - EUROfusion; WP07: ENR-DeHydroc-1,2,3_HE-FU
   Andreja Šestan Zavašnik, B. Sc.
   European Commission

R&D GRANTS AND CONTRACTS

1. Nanoscale investigations of diffusion controlled topotaxial phase transformations in rutile-corundum host systems
   Dr. Sandra Drev
2. Detection of defects and hydrogen by ion beam analysis in channelling mode for fusion
   Andreja Šestan Zavašnik, B. Sc.
3. External Services (Export), Electron Microscopy and Microanalysis, Sample Preparation and Microscopy
   Prof. Miran Čeh

NEW CONTRACT

1. BIO1-2020
   Prof. Miran Čeh
   Lek d. d.

STAFF

Researcher
1. **Prof. Miran Čeh, Head**
Postdoctoral associate
2. Dr. Sandra Drev
Postgraduates
3. Andreja Šestan Zavašnik, B. Sc.

4. Aleksander Učakar, B. Sc.
Technical officers
5. Dr. Jitka Hreščak
6. *Maja Koblar, B. Sc., 01.09.21, transferred to Department K5*

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2. Stefan Schymura *et al.* (11 authors), "Dissolution-based uptake of CeO_2 nanoparticles by freshwater shrimp: a dual-radiolabelling study of the fate of anthropogenic cerium in water organisms", *Environmental science: Nano*, 2021, **8**, 7, 1934-1944.
3. Matic Korent, Marko Soderžnik, Urška Ročnik, Sandra Drev, Kristina Žužek Rožman, Sašo Šturm, Spomenka Kobe, Kristina Žagar, "Toward low-energy spark-plasma sintering of Hot-deformed Nd-Fe-B magnets", *International journal of materials science and applications*, 2021, **10**, 5, 98-107.
4. Petra Jenuš, Aleksander Učakar, Sandra Repše, Claudio Sangregorio, Michele Petrecca, Martin Albino, Riccardo Cabassi, César De Julián Fernández, Blaž Belec, "Magnetic performance of $SrFe_{12}O_{19} - Zn_{0.2}Fe_{2.8}O_4$ hybrid magnets prepared by Spark Plasma Sintering", *Journal of physics. D, Applied physics*, 2021, **54**, 20, 204002.
5. Tjaša Gornik, Sudhirkumar Shinde, Lea Lamovšek, Maja Koblar, Ester Heath, Börje Sellergren, Tina Kosjek, "Molecularly imprinted polymers for the removal of antidepressants from contaminated wastewater", *Polymers*, 2021, **13**, 1, 120.

INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Janez Zavašnik, Andreja Šestan, Vasyl Shvalya, "Microscopic techniques for the characterisation of metal-based nanoparticles", In: *Analysis and characterisation of metal-based nanomaterials*, (Comprehensive analytical chemistry **93**), Elsevier, 2021, 241-284.
2. Janez Zavašnik, Andreja Šestan, Vasyl Shvalya, "Microscopic techniques for the characterisation of metal-based nanoparticles", In: *Analysis and characterisation of metal-based nanomaterials*, (Comprehensive analytical chemistry **93**), Elsevier, 2021, 241-284.

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 a direct exchange of information and experience between researchers and the users of their research results. The centre has thirteen researchers and technicians working in the areas of research results' dissemination and eLearning. In particular, the centre is well known for its portals: VideoLectures.NET with multimedia materials of numerous scientific events, on-line training materials, and a collection of tutorials on different scientific fields; ScienceAtlas.ijs.si and IST-World.Org for analysis and visualization of large bibliographic and project databases. The centre covers management, training and dissemination activities of several EU projects.

Head:

Mitja Jermol, M. Sc.

In 2021 we were active in the following projects within the H2020 program: *WATER4CITIES (Holistic Surface Water and Groundwater Management for Sustainable Cities); ELEXIS (European Lexicographic Infrastructure); SILKNOW (Silk Heritage in the Knowledge Society: from punched cards to big data, deep learning and visual/tangible simulations); COG-LO (COGnitive Logistics Operations trough secure, dynamic and ad-hoc collaborative networks); CyberSANE (Cyber Security Incident Handling, Warning and Response System for the European Critical Infrastructures); NAIADES: A Holistic Water Ecosystem for Digitisation of Urban Water Sector; INFINITECH (Tailored IoT & BigData Sandboxes and Testbeds for Smart, Autonomous and Personalized Services in the Europe); FACTLOG (Energy-Aware Factory Analytics for Process Industries), A-CINCH: Augmented Cooperation in Education and Training in Nuclear and Radiochemistry; EU-Japan.AI (Advancing Collaboration and Exchange of Knowledge Between the EU and Japan for AI-Driven Innovation in Manufacturing); STAR (Save and Trusted Human Centric AI Future Manufacturing Lines); ODEUROPA (Negotiating Olfactory and Sensory Experiences in Cultural Heritage Practice and Research); ERASMUS+: QALead (Equipping Institutional Leaders to Maximise Gains from Quality Assurance) and BRIDGES (Bridging Educational Emergency to Digital Pedagogies).*

In 2021 we participated in fourteen European projects.

The centre prepares and organizes educational events, such as conferences, seminars, workshops and summer schools. These are targeted at experts who would like to apply the latest knowledge and achievements of intelligent data analysis, knowledge technologies, data mining, text mining and decision support to the areas of network organizations, business decisions, finance and marketing. Special consideration is put on the managers and decision makers who are aware of the strengths and benefits of the success of their business. All educational events are designed to transfer basic, additional and latest expert knowledge to the companies, research and educational organizations.

To make the knowledge transfer efficient, we combine the traditional and ICT-supported training methods. For this purpose, we run a number of training web portals. The most popular one is http://videolectures.net/. It now offers 28.655 recorded tutorials from different scientific events. The main purpose of the portal is to provide free and open access to high-quality video lectures presented by distinguished scholars and scientists at the most important and prominent events. In today's world, VideoLectures.NET presents a free knowledge hub, a way of opening up education to everyone as there is a great need to share educational content at all levels in order to benefit society and foster economy. It gives a learning opportunity to audiences of all social groups.

We provided technological support to scientific conference organizers by enabling them to post pre-recorded content and moderate the use of its online tools such as Zoom, Skype or the Slovenian MiTeam platform where we took care of video playback. We provided nearly 40 live streams. The events we filmed were mostly hybrid, meaning part live and part online. This allowed thousands of viewers to participate live and moderate questions about the interactive content. Using technical guidance on how to use the tools that are regularly available to everyone,

Figure 1: Participants of OE4BW in 2021/22

we organised many international and national conferences where we also secured the appropriate consents and enabled the reliability of the content with certain video materials. The biggest events prepared in 2021 were: the ISWC 2021 Conference, 6th Symposium of Slovenian Researchers Abroad, Physics of the Flavorful Universe, European Mathematics Congress 2021, 30th Web Conference VIRTUAL EDITION and others.

We also continued to collaborate on projects such as A-CINCH and cultivated long-term partnerships. Videolectures continued to be included in IJS seminars, Faculty of Architecture lectures, the series of Science on the Road lectures, the series of Positive Psychology lectures, and the lectures for schools or parents. We started recording interesting literary evenings at the Konzorcij bookstore in Ljubljana. We also filmed and presented the professional basis for Slovenia's long-term climate strategy until 2050.

Videolectures.Net released a VLN app for cell phones, which is already publicly available but is still being developed. We provided dissemination channels for the Water4Cities project and participated in the research and training activities at the project coordinator's facility.

In the spring of 2021, due to the situation related to the COVID pandemic, we again organized and carried out the 16th ACM Competitions in Computer Science and Informatics. All competitors were simultaneously given access to the competition systems of ACM Slovenia (https://rtk.fri.uni-lj.si/ and https://putka-rtk.acm.si/), while having competitions all the time as all questions were also available to the Organizing Committee and the Commission for the Competition in Computer Science and Informatics. 164 students from 27 high schools participated in the field of computer science skills (programming), 12 students competed in the field of online application development, and 4 participants took the challenge in an offline task. Every year we also receive quite a few instructional videos; this time there were two videos from elementary schools and twenty-two videos from secondary schools. The results of the competition are available at https://rtk.ijs.si/2021/rezultati.html. Each year we also award practical prizes to the best participants. A total of 209 students from all over Slovenia participated in the school programming contest held in January.

Figure 2: OE4BW Eduscope 2021 logo

In 2021 we ran the international mentoring program "Open Education for a Better World" for the fourth time. The work took place at three regional hubs, namely "North and South America", "Africa and Europe", and "Asia", as well as five thematic hubs, namely "Field Education", "Science, Technology, Engineering, Mathematics and Medicine", "Energy, Biodiversity, Sustainability", "Society, Peace, Justice, Equality" and, for the first time, the "Youth Hub". The online event "OE4BW Eduscope" organised in the autumn was attended by 400 experts from 36 countries and six continents.

In 2020/21, the 4th year of the international mentoring program "Open Education for a Better World" was managed by the UNESCO Chair on Open Technologies for Open Educational Resources, the Open Learning Jožef Stefan Institute and the University of Nova Gorica. We received more than 100 applications and therefore organized 3 regional hubs – Hub "North and South America"; Hub "Africa and Europe"; Hub "Asia" – and five thematic hubs – Hub "Field Specific Education"; Hub "Science, Technology, Engineering, Mathematics and Medicine (STEMM)"; Hub "Energy, Biodiversity, Sustainable Living"; Hub "Society, Peace, Justice, Gender, Equity" and Hub "Youth". In the scope of the programme we also organised webinars in the fields of open education, open pedagogy and open education policy.

On 18–21 October 2021 we organized an online event called "OE4BW Eduscope 2021", which took place entirely online at the MiTeam platform. The event was attended by 400 participants from 36 countries and 6 continents.

We started 2022 with as many as 60 project proposals from 97 developers due to many group applications. More information about the programme, projects, developers and mentors is available at https://oe4bw.miteam.si/

In September 2021 we concluded, together with the Water4Cities (Integrated Surface and Groundwater Management for Sustainable Urban Development), another project under the EU Horizon 2020, and the Marie Skłodowska Curie RISE project, carried out together with the Artificial Intelligence Laboratory. We finished the data analysis on groundwater, rivers and stormwater flow in the Ljubljana aquafier, and on the water quality and consumption on the Greek island of Skiathos. We developed a model that

Figure 3: CT3 and E3 teams with the Water4Cities coordinator at the Eighth International Conference on Environmental Management, Engineering, Planning and Economics (CEMEPE 2021) and SECOTOX Conference 2021

allows us to monitor the optimal water management in real time. We attended the "Eighth International Conference on Environmental Management, Engineering, Planning and Economics (CEMEPE 2021) and SECOTOX Conference 2021", which took place on 20–24 July 2021 in Thessaloniki, Greece. The Water4Cities consortium organized a

special session where the project results were presented. In 2021 we published regular webinars, available, together with all the other project video material, on the Videolectures.NET subpage – http://videolectures.net/water4cities/.

The EU H2020 COG-LO project (COGnitive Logistics Operations through secure, dynamic and ad-hoc collaborative networks) ended last year and the aim to create a framework and tools that add cognition and collaborative features to future logistics processes was achieved. Together with the Department for Artificial Intelligence (E3), we were involved in the design and development of the tool "Cognitive Advisor", which realizes the cognitive behaviour of a Cognitive Logistics Object (CLO) based on the reference implementation model. We were also involved in project pilots, especially in the pilot with postal operators (Slovenian and Croatian Post). The project included data streams that helped define the necessary cognitive methods and optimization algorithms. Within dissemination activities, we created promotional videos presenting the pilots and the developed solution.

The EU H2020 INFINITECH project (Tailored IoT & BigData Sandboxes and Testbeds for Smart, Autonomous and Personalized Services in the European Finance and Insurance Services Ecosystem) aims to lower the barriers for BigData/IoT/AI-driven innovation and boost regulatory compliance in the financial and insurance sector. Together with the Department for Artificial Intelligence (E3), we are involved in the pilot that develops a platform for the improvement of the effectiveness of the existing supervisory activities in anti-money laundering and combating terrorist financing (AML/ CTF) by processing large quantities of data (Big Data) owned by the Bank of Slovenia

Figure 4: Working in special COVID conditions

(BS) and other competent authorities. Moreover, INFINITECH established a market platform that provides access to project solutions, along with a Virtualized Digital Innovation Hub (VDIH) that supports innovators (FinTech/ InsuranceTech) in their BigData/AI/IoT endeavours.

The CyberSANE project (Cyber Security Incident Handling, Warning and Response System for the European Critical Infrastructures) started in 2019 and aims to increase the security and resilience of the European Critical Information Infrastructure (CII). As part of the project, we are developing a CyberSANE platform to help professionals in organizations deal with cyber incidents.

The platform consists of several components, and in 2021 we were responsible for the development of the DarkNET component, enabling the capture and analysis of structured and unstructured data from the so-called dark web as well as from media articles. In 2021 the development of the component was completed, and the component is currently being implemented on the CyberSANE platform. The component is used for the creation of reports and alerts on detected cyber threats from the dark web and the news.

In 2021 we also started preparing an educational publication in English for the requirements of the project – a manual whose goals are to provide a clear overview of the various aspects of information security relevant for business entities and to provide technologically neutral advice for the implementation of the protection against cyber-attacks within companies. The handbook is intended for managers and employees working at the organisations operating in the field of critical infrastructure.

In January we started working at the new project named EU-Japan.AI. This project aims to establish and stimulate a long-term cooperation between EU and Japan in the areas relevant to AI-driven innovation in manufacturing and digital industry, by implementing a platform-based approach to connect all the relevant stakeholders and by promoting the use of modern, online-driven awareness approaches to them.

Within the project we collect data about relevant events, projects, organizations and opportunities in the EU and Japan in the area of AI in manufacturing. This information is published on a web portal, with the goal to connect partners from both regions and foster cooperation among them.

In the initial phase the project partners collected the data manually, collecting secondary data (the so-called "desk research"). However, at the JSI we are developing tools for automatic collection and processing of data in text form, so we have started to develop the so-called EUJapan Observatory. It is a tool that automatically collects data on scientific publications in the field of artificial intelligence and media reports on the events related to artificial intelligence. We then analyse these data with our tools and present comparative analyses on the EUJapan Observatory website. In the coming months we will also implement the data collection and analysis of the job market and data on the demand for skills in the field of artificial intelligence. We also intend to include the data on research projects and open-source projects related to artificial intelligence in the Observatory. Finally, we are preparing a visualization and analysis of artificial-intelligence public policies for both regions.

Organization of conferences, congresses and meetings

1. 16th Student competition in computer science, Ljubljana, Ljubljana, 27. 3. 2021 (virtual)
2. Organization of the event OE4BW Eduscope 2021, 18. – 21. 10. 2021 (virtual)
3. Organization and implementation of the "Training for the implementation of distance learning and the production of free available educational materials", 11.15.-11.19.2021 (virtual)

INTERNATIONAL PROJECTS

1. INEA/CEF - MARCELL, Multilingual Resources for CEF.AT in the Legal Domain
   Mitja Jermol, M. Sc.
   Innovation And Networks Executive Agency (inea)
2. ERASMUS+; MentorTrain - Training and Equipping Mentors in SMEs to provide Quality Apprenticeships
   Mihajela Črnko
   European Commission
3. ERASMUS+: QALead - Equipping Institutional Leaders to Maximise Gains from Quality Assurance
   Matija Ovsenek
   European Commission
4. ERASMUS+: BRIDGES - Bridging Educational Emergency to Digital Pedagogies
   Anja Polajnar, M. Sc.
   Agenzia Nazionale Erasmus Plus Indire
5. COST CA19142; Leading Platform for European Citizens, Industries, Academia and Policymakers in Media Accessibility
   Davor Orlić, B. Sc.
   Cost Association Aisbl
6. H2020 - Water4Cities; Holistic Surface Water and Groundwater Management for Sustainable Cities
   Mitja Jermol, M. Sc.
   European Commission
7. H2020 - SILKNOW; Silk Heritage in the Knowledge Society; From Punched Cards to Big Data, Deep Learning and Visual/Tangible Simulations
   Mitja Jermol, M. Sc.
   European Commission
8. H2020 - COG-LO; COGnitive Logistics Operations through secure dynamic and ad-hoc collaborative networks
   Mitja Jermol, M. Sc.
   European Commission
9. H2020 - EnviroLENS; Coprenicus for Environmental Law Enforcement Support
   Mitja Jermol, M. Sc.
   European Commission
10. H2020 - FIN-TECH; A FINancial supervision and TECHnology compliance training programme
    Mitja Jermol, M. Sc.
    European Commission
11. H2020 - NAIADES; A Holistic Water Ecosystem for Digitisation of Urban Water Sector
    Mitja Jermol, M. Sc.
    European Commission
12. H2020 - CyberSANE; Cyber Security Incident Handling, Warning and Response System for the European Critical Infrastructures
    Mitja Jermol, M. Sc.
    European Commission, the Directorate-General
13. H2020 - INFINITECH; Tailored IoT&BigData Sandboxes and Testbeds for Smart, Autonomous and Personalized Services in the European Finance and Insurance Services Ecosystem
    Mitja Jermol, M. Sc.
    European Commission
14. H2020 - FACTLOG; Energy-aware Factory Analytics for Precess Industries
    Mitja Jermol, M. Sc.
    European Commission
15. H2020 - A-CINCH; Augmented Cooperation in Education and Training in Nuclear and Radiochemistry
    Mihajela Črnko
    European Commission
16. H2020 - STAR; Safe and Trusted Human Centric Artifical Intelligence in Future Manufacturing Lines
    Mitja Jermol, M. Sc.
    European Commission
17. H2020 - ODEUROPA: Negotiating Olfactory and Sensory Experiences in Cultural Heritage Practice and Research
    Mitja Jermol, M. Sc.
    European Commission
18. H2020 - EU-Japan.Ai: Advancing Collaboration and Exchange of Knowledge Between the EU and Japan for AI-Driven Innovation in Manufacturing
    Mitja Jermol, M. Sc.
    European Commission
19. H2020 - ELEXIS; European Lexicographic Infrastructure
    Mitja Jermol, M. Sc.
    European Commission

R&D GRANTS AND CONTRACTS

1. IRCAI - International Research Center for Artificial Intelligence – UNESCO
   Mitja Jermol, M. Sc.
   Ministry of Education, Science and Sport
2. Videorecording and Post-Processing
   Mitja Jermol, M. Sc.
3. Recording, Publishing and Disseminating of the Scientific Content of the EnetCollect Project on Videolectures.net
   Mihajela Črnko
   Eurac Research
4. Management of the European Statistics Award for Web Intelligence - LOT 1
   Anja Polajnar, M. Sc.
   European Commission
5. Management of the European Statistics Award for Nowcasting - LOT 2
   Anja Polajnar, M. Sc.
   European Commission
6. TIDES: Connect AI
   Mitja Jermol, M. Sc.
   Tides Foundation

STAFF

Postdoctoral associate
1. *Ayse Saliha Sunar, B. Sc., left 01.06.21*
Postgraduate
2. Anja Polajnar, B. Sc.
Technical officers
3. **Mitja Jermol, M. Sc., Head**
4. Dr. Matej Kovačič
5. Simon Marolt, B. Sc.
6. Dr. Tanja Zdolšek Draksler

Technical and administrative staff
7. Aleš Buh
8. *Mihajela Črnko, 01.08.21, transferred to Department E3*
9. Ana Fabjan, B. Sc.
10. Adis Krečo, B. Sc.
11. Monika Kropej, B. Sc.
12. Matija Ovsenek
13. *Kim Sevšek, B. Sc., 01.08.21, transferred to Department E3*
14. Špela Sitar, B. Sc.

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Original Article

1. Tanja Zdolšek Draksler, Karin Širec, "The study of entrepreneurial intentions and entrepreneurial competencies of business vs. non-business students", *Journal of Competitiveness*, 2021, **13**, 2, 171-188.

Independent Component Part or a Chapter in a Monograph

1. Aitor Apaolaza *et al.* (27 authors), "MOVING: a user-centric platform for online literacy training and learning", In: *e-Science: open, social and virtual technology for research collaboration*, (Progress in IS), Springer, 2021, 77-130.

MILAN ČOPIČ NUCLEAR TRAINING CENTRE ICJT

The mission of the ICJT training centre is training in the field of nuclear technologies and radiation protection. In addition, ICJT is actively informing the public about those technologies.

In 2021 the activity of ICJT was already well adapted to the Covid-19 pandemic. Through the implementation of protective measures (face masks, ventilation, hand sanitation), the majority of training was held live in classrooms and laboratories, naturally with a limited number of participants and sufficient distance between tables. The visits of school groups were mainly done using a videoconference system. Occasionally some participants or lecturers had to stay at home because they were infected or in quarantine, and in these cases, they were connected by computer and were following the lectures or taking the exam remotely. We are proud that there was not a single case of infection transfer during the training process at the ICJT.

Training in the area of nuclear technologies is our primary mission. The *Nuclear technology* (TJE) course is the first, theoretical phase of training for future control-room operators and was held from September to February 2022. We also conducted three 2-month courses *Basics of nuclear technology* (OTJE); the two such courses in June and July were held in parallel (with 2-week delay) to keep the number of participants in one group sufficiently small. Despite occasional use of the videoconference system, all these courses were concluded in the anticipated time frame. In addition to these "classic" courses, there were also two courses for Slovenian nuclear safety administration (*Selected chapters of Nuclear Technology* and *Nuclear technology fundamentals*) and two courses *Nuclear Energy in Short*.

Head:
Dr. Igor Jenčič

Intensive training in the area of nuclear technologies took place in 2021. In addition to the Nuclear technology course there were 3 courses Basics of nuclear technology and 4 other courses.

There were 31 **radiological protection training** courses for the medical, industrial and research use of radioactive sources.

In collaboration with the Reactor Physics Division and the Reactor Infrastructure Centre three **international courses** were organized.

Public information remains an important part of our activities. Due to the pandemic, there were significantly fewer live visits to our information centre, which was in part replaced by lectures and workshops over a videoconference system. The lectures were offered on electricity from nuclear energy, fusion, isotopes, energy in general, and the use of radiation in industry, medicine and research. Altogether, there were 98 groups with a total of 2935 participants this year. Since 1993, there were 192,705 pupils, teachers and others, that visited our information centre. We have continued monitoring and analysing media reports on nuclear energy.

Figure 1: Implementation of a lecture via the videoconference system Zoom, for students of Gabrovka primary school.

Figure 2: Training session at the Basics of Nuclear Technology course

STAFF

Researcher
1. **Dr. Igor Jenčič, Head**
Technical officers
2. Sara Gregl, B. Sc.
3. Matjaž Koželj, M. Sc.
4. Urban Pompe, B. Sc.

5. Tomaž Skobe, M. Sc.
6. Vesna Slapar Borišek, B. Sc.
Technical and administrative staff
7. Saša Bobič
8. Matejka Južnik, M. Sc.
9. Borut Mavec, B. Sc.

Table of training activities at the Nuclear Training Centre in 2021

Date	Title of the course	Partici-pants	Lecturers	Weeks	Participants × weeks
12. - 19.1.	Radiation protection for RP department staff - refresher course	12	1	0.4	4.8
29.1.	Radiation protection for baggage screening systems - refresher course	5	2	0.2	1
25.2.	Radiation protection for exposed workers in Krško Nuclear Power Plant - Refresher Course	2	2	0.2	0.4
1. - 3.3.	Radiation protection for handheld XRF spectroscopy	18	3	0.6	10.8
1. - 3.3.	Radiation protection for industrial and other practices (measurement of road-way density and humidity)	1	3	0.6	0.6
1. - 18.3.	Radiation protection for industrial and other practices (radiography)	2	3	1	2
8.3.	Radiation protection for baggage-screening systems	1	3	0.2	0.2
8.3.	Radiation protection for industrial and other practices	4	3	0.2	0.8
8. - 9.3.	Radiation protection for industrial and other practices (unsealed sources)	1	4	0.4	0.4
8. - 11.3.	Radiation protection for Nuclear Medicine Dept.	13	7	0.8	10.4
11.3.	Radiation protection for industrial and other practices - Refresher Course	6	3	0.2	1.2
11.3.	Radiation protection for industrial and other practices (measurement of road-way density and humidity) - Refresher Course	3	3	0.2	0.6
11.3.	Radiation protection for industrial and other practices (unsealed sources) - Refresher Course	4	4	0.2	0.8
11. - 12.3.	Radiation protection for industrial and other practices (radiography) - refresher course	7	3	0.4	2.8
17.3.	Radiation protection for industrial and other practices - Refresher Course	9	3	0.2	1.8
7.5.	Radiation protection for baggage screening systems - refresher course	5	2	0.2	1
10.5. - 9.6.	Basics of nuclear technology, theory	15	11	4.2	63
24.5. - 23.6.	Basics of nuclear technology, theory	13	13	4.4	57.2
9.6. - 2.7.	Basics of nuclear technology, systems	17	8	3.4	57.8
23.6. - 16.7.	Basics of nuclear technology, systems	12	8	3.4	40.8
5. - 13.7.	Activities on nuclear instrumentation and research reactor	14	7	1.4	19.6
31.8. - 3.9.	Nuclear technology fundamentals	6	7	0.8	4.8
13.9. - (4.2.22)	Nuclear Technology, Theory	12	18	15.6	187.2
20. - 22.9.	Radiation protection for High-Activity Sealed Sources - Refresher Course	1	3	0.6	0.6
20. - 22.9.	Radiation protection for handheld XRF spectroscopy	3	3	0.6	1.8
20. - 24.9.	Radiation protection for industrial and other practices (radiography)	2	3	1	2
27.9.	Radiation protection for baggage-screening systems	1	3	0.2	0.2
27.9.	Radiation protection for industrial and other practices	11	3	0.2	2.2
27. - 30.9.	Radiation protection for Nuclear Medicine Dpt.	8	7	0.8	6.4
27.9. - 1.10.	Uppsala University Dedicated Practical Educational Course "Experimental reactor physics"	5	3	1	5
30.9.	Radiation protection for industrial and other practices - Refresher Course	13	3	0.2	2.6
30.9.	Radiation protection for industrial and other practices (unsealed sources) - Refresher Course	3	4	0.2	0.6
30.9.	Radiation protection for workers exposed to radon and thoron	1	4	0.2	0.2
30.9.	Radiation protection for handheld XRF spectroscopy - Refresher course	5	3	0.2	1

Table of training activities at the Nuclear Training Centre in 2021

Date	Title of the course	Partici-pants	Lecturers	Weeks	Participants × weeks
30.9. - 1.10.	Radiation protection for industrial and other practices (radiography) - refresher course	5	3	0.4	2
13. - 18.10.	Nuclear Energy in Short	10	5	0.6	6
18.10.	Radiation protection for industrial and other practices - Refresher Course	15	2	0.2	3
27.10.	Radiation protection for exposed workers in Krško Nuclear Power Plant - Refresher Course	5	2	0.2	1
2. - 5.11.	Selected chapters of Nuclear Technology	7	5	0.8	5.6
8. - 10.11.	Nuclear Energy in Short	17	4	0.6	10.2
12.11.	Radiation protection for industrial and other practices	5	1	0.2	1
15.11. - 15.12.	Basics of nuclear technology, theory	7	13	4.4	30.8
15.12 - (14.1.22)	Basics of nuclear technology, systems	7	8	4.2	29.4
17.12.	Pulse experiment exercise for students	22	5	0.2	4.4
17.12.	Radiation protection for industrial and other practices	7	2	0.2	1.4
TOTAL		342	210	56.4	587.4

Figure 3: Trainees in the lecture room during of the Basics of Nuclear Technology course, December 2021

Figure 4: Group photograph of trainees and lecturers at the conclusion of the Nuclear Technology course

R&D GRANTS AND CONTRACTS

1. Strengthening the Competence of Entrepreneurship and Promoting Flexible Transition between Education and the Environment in Primary and lower Secondary Schools
   Tomaž Skobe, M. Sc.
   Ministry of Education, Science and Sport
2. Strengthening the Competence of Entrepreneurship and Promoting Flexible Transition between Education and the Environment in Secondary Schools
   Tomaž Skobe, M. Sc.
   Ministry of Education, Science and Sport
3. Services
   Matejka Južnik, M. Sc.
4. Training Courses TJE and OTJE - For Foreign Participants
   Dr. Igor Jenčič

NEW CONTRACTS

1. Preparation of training materials for the NEK Safety Upgrade Program
   Dr. Igor Jenčič
   Krško Nuclear Power Plant, Krško
2. Services
   Matejka Južnik, M. Sc.
3. Trainings of the Radiation protection
   Matejka Južnik, M. Sc.
4. Operation of the Nuclear Information Centre in 2021
   Dr. Igor Jenčič
   Gen energija, d.o.o.
5. Basic Training Course on Nuclear Technology and Nuclear Power Plants
   Dr. Igor Jenčič
6. ICJT Training Programme implementation in the year 2021
   Dr. Igor Jenčič
   Krško Nuclear Power Plant, Krško

RADIATION PROTECTION UNIT

SVPIS

SVPIS has been involved in ionizing-radiation measurements and radiation protection since the commissioning of the TRIGA MARK II Research Reactor in 1966. SVPIS is responsible for the radiation control of all the activities at the Institute dealing with ionizing radiation. Our main task is the supervision of work in the reactor with the Hot-Cell Facility, and we are authorised by the regulatory authority to perform environmental monitoring.

SVPIS also controls 17 laboratories that use sources of ionising radiation in their research work. There are different sources of radiation used, such as sealed sources, open sources, X-ray units and the TANDETRON accelerator, which need regulatory control. Furthermore, we are involved in radioactive-waste management.

SVPIS is authorized by the Slovenian radiation-protection administration and nuclear safety administration to perform control in industrial and research institutions dealing with open or sealed radioactive sources and X-ray units.

The measurements of dose rate, contamination, gamma spectrometry and radon activity concentration are performed by accredited methods (LP-022, EN ISO/IEC 17025).

Head:
Matjaž Stepišnik, M. Sc.

Personal dosimetry

Personal doses of 135 workers that regularly or occasionally deal with ionizing radiation were monitored with Thermo Luminescent Dosimeters. The maximum individual yearly dose was 0.52 mSv. This is 3 % of the regulatory limit for occupational exposure (20 mSv per year). The collective dose at the JSI in 2021 was 4.7 man mSv.

Supervision of research reactor and laboratories

The controlled area of the Research Reactor, the Hot Cell Facility and the Department of Environmental Sciences was monitored on a weekly basis. During some activities the constant presence of a radiation-protection worker was needed (i.e., for the opening of activated samples or radioactive-waste management). Measurements of dose rate, surface contamination, contamination of different objects and personal contamination were performed routinely. In most cases, no or very low contamination levels were measured. Locally elevated radiation levels could be measured mostly in the reactor's controlled area.

At present, 104 radioactive sources (open and sealed) and devices with ionizing radiation (X-ray units and accelerator TANDETRON) sources of radiation are in use, which require regulatory control and additionally 450 low-activity sources in different laboratories.

In 2021, 21 radiological surveys in other JSI laboratories were performed. An independent inspection by an external authorized institution was performed in the SVPIS laboratory and two additional laboratories at the JSI. There were no deficiencies recognized that could be important for radiation protection.

Environmental monitoring of the reactor

The environmental monitoring of the Reactor Center was performed according to the existing programme. The programme consists of effluent measurements and measurements of samples in the environment. Activity concentrations of gamma emitters in water samples, filters, noble gases, soil samples and sediment samples were measured periodically. About 500 different samples for the reactor and different laboratories have been measured with gamma spectrometry. Environmental passive dosimeters have been used to monitor the 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. **In 2021 the public exposure due to activities at the Reactor Center was insignificant**.

Expert assessments and measurements for outside customers

The Radiation Protection Unit is authorized for supervision measurements and expert assessments in the field of radiation protection. In the past year several radiological control investigations were carried out in industrial and research institutions (in total 39). Our group has participated in the evaluation of the radiological monitoring of Krško NPP, research reactor TRIGA and storage for low- and intermediate-level waste in Brinje.

Jožef Stefan Institute

STAFF

Technical officers
1. Dr. Tinkara Bučar
2. Mitja Eržen, B. Sc.
3. **Matjaž Stepišnik, M. Sc., Head**

Technical and administrative staff
4. Thomas Breznik, B. Sc.
5. Jasna Kopač, B. Sc.
6. Tanja Murn, B. Sc.
7. Nina Udir, B. Sc.

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INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Matjaž Stepišnik, "Radioaktivnost v rečni vodi, sedimentih in ribah", In: *Ovrednotenje meritev radioaktivnosti v reki Savi, pitni vodi, padavinah, zraku, zemlji in hrani v okolici NEK in po Sloveniji*, Institut "Jožef Stefan", 2021, 106-1-106-19.

PROFESSIONAL MONOGRAPH

1. Matjaž Stepišnik, Jasmina Kožar Logar, Toni Petrovič, Marko Giacomelli, Matjaž Korun, Katarina Vogel-Mikuš, *Ovrednotenje meritev radioaktivnosti v reki Savi, pitni vodi, padavinah, zraku, zemlji in hrani v okolici NEK in po Sloveniji*, Institut "Jožef Stefan", 2021.

CENTER FOR TECHNOLOGY TRANSFER AND INNOVATION   CTT

The Technology Transfer Office was established in 1996 and transformed in January 2011 when an independent Center for Technology Transfer and Innovation (CTT) was created to continue within the third-pillar mission at the Jožef Stefan Institute (JSI). We assist in the process of technology and knowledge transfer from the JSI to industry, which includes licensing, spin-out creation and associated procedures for the protection of intellectual property. We assist companies by finding suitable local and international research partners for contract and collaborative research. We also support knowledge transfer from science to the school system and promote the recognition of the JSI as well as science in general among young people and the wider public.

Head:
Dr. Špela Stres, MBA, LLM

The center's success is based on 13 professionals, 6 of whom hold degrees in natural sciences and engineering, 9 in economics, 1 in law. One of the experts is also qualified as a patent attorney and a Registered Technology Transfer Professional (RTTP). The head of the center is a member of the first European Innovation Council steering board. We are members of the ASTP (Association of Science and Technology Professionals), the LES (Licensing Executives Professionals), the Association of Technology Transfer Professionals, the Association of Slovenian Patent Attorneys, while three team members hold a U. S. Certified Licensing Professional certificate.

We have created a network of contacts with enterprises and other organizations in Slovenia and abroad. **Our services**, fine-tuned towards individual needs, include analyses of requirements, preparation, registration and protection of intellectual property, marketing of intellectual property (including secret know-how), identification of negotiation points, carrying out negotiations, drafting of various agreements, creation of spin-out companies, access to information and research infrastructure, and support in establishing financial measures. **Our clients** are primarily JSI researchers, although numerous companies and other research organizations also procured our services in 2021.

In 2021, the CTT faced several activity-related **challenges**, the biggest of which were:

(i)   the content-based upgrade of financial consulting for the SME-PRO collaboration;

(ii)   the second Innovation Fund (Proof-of-Concept) call at the JSI, and

(iii)   raising awareness at the JSI about CTT activities within the third-pillar mission.

In 2021 we continued our support to SMEs seeking funding for collaborating with researchers, particularly in the income tax deduction. In 2021 we continued with the Proof-of-Concept Innovation Fund initiative, resulting in funding of five successful JSI research projects to increase the technology readiness level (TRL). In 2021 we presented CTT activities and initiatives to commercialize JSI assets (such as research equipment) at JSI expert councils. We again participated in the section on research in the field of technology transfer at the International Technology Transfer Conference, thereby raising the context of technology transfer to a level of scientific discourse.

Despite the epidemiological situation in 2021, we managed to perform our services thoroughly and without significant obstacles. We organized the International Technology Transfer Conference as well as company visits and school visits, partly or entirely online.

In 2021 the Center for Technology Transfer and Innovation was partly funded through **two larger and two smaller European and national projects**. Our projects were run under various funding programs and schemes. These included the Enterprise Europe Network (EEN) Slovenia

Figure 1: Winners of the Prize for best innovations from public research organizations (photo: M. Verč)

- Preparation, protection and marketing of 23 JSI technologies; 132 identified RR topics; 16 license and 22 research-and-development agreements signed with domestic and foreign companies.
- Second Proof-of-Concept Innovation Fund call; funding of five JSI research projects for increasing the TRL technology in the amount of 42,042.42 euros.
- JSI research capacities and technologies presented at 47 company visits.
- JSI researchers informed about 1600 relevant domestic and international project calls. Assistance in seeking partners for 30 project applications. Assistance in the preparation of 17 applications.

(COSME scheme), KET4Clean Production (Horizon 2020) as well as the national projects KTT (MIZŠ) and Intellectual Property Valorization (ARRS CRP). Project activities were combining and complementing our core TT activities. Within the KTT project, we coordinate the Consortium for Technology Transfer from PROs to industry, including the largest Slovenian public research organizations. Within the EEN project, we coordinate the Slovenian branch of the Enterprise Europe Network.

CTT is divided into four groups whose activities interact with and complement each other.

GROUP FOR THE PROTECTION AND MARKETING OF INTELLECTUAL PROPERTY processes **IP protection and marketing** cases that are submitted through the single entry point, arranges introductory meetings with researchers (23) and prepares patentability assessments, including in-depth state-of-the-art analyses (5). The group also conducts detailed market potential analyses (4), helps develop the invention description for disclosure within the Institute (5), helps fulfil the terms for patent application filing, prepares agreements on the ownership of intellectual property (7), searches for suitable patent attorneys for filing and processing the applications (18), and advises about the strategy of international and national expansion of the patent protection. The group also carries out passive marketing: 12 technology profiles were promoted through the Enterprise Europe Network, 74 expressions of interests were received, and active marketing: the above-mentioned technologies were promoted directly to more than 700 companies and other organizations, with 14 expressions of interests received. Moreover, group members arrange signatures of non-disclosure agreements (13), take part in negotiations, and prepare and close license (16) or research and development (22) agreements.

Figure 2: Recipients of the World Intellectual Property Organization awards – WIPO Medal for Inventors, and WIPO Enterprise Trophy (photo: M. Verč)

- **Organization of the 14th International Technology Transfer Conference. More than 140 visitors. The competition for the best innovation; two ITTC best innovation awards, two WIPO awards – the WIPO Medal for inventors, recognizing researchers for their impact on society, and the WIPO IP Enterprise Trophy for a company most efficiently utilizing and promoting intellectual property.**
- **13th award ceremony for the best innovation with market potential; a total of more than 58.000 euros awarded since the first International Technology Transfer Conference.**
- **Continued inclusion of the section on research in technology transfer in the International Technology Transfer Conference, expanding the scope of technology transfer to the level of scientific discourse.**

Group members also provided individual consulting for all the phases of a **spin-out** company's creation (12). They helped with the preparation of business plans, defined interest for the use of intellectual property, equipment and facilities at the JSI, contacted external mentors and supporting programmes, informed and contacted financing sources, managed discussions on the arrangement of the relationship between the JSI and researchers within entrepreneurial teams, prepared documentation for spin-out creation, helped valorize the intellectual property, prepared agreements for access to the infrastructure and prepared license agreements for the use of technology within a spin-out company.

The group actively sets up and plans collaboration with actors that are setting up a regional venture capital fund in excess of 40 million euros, which is being built by the European Investment Fund in collaboration with the Slovenian and Croatian investment banks (SID and HBOR, respectively). The fund will represent an important addition to the financial sources for spin-out companies from Slovenian and Croatian PROs, which previously have not had this opportunity.

The group set up collaboration with the Ljubljana MBA Programme, within which a spin-out team with members from the JSI and the National Institute of Biology, Faculty of Mechanical Engineering at the University of Ljubljana, collaborated with a group of 9th generation MBA students and mentors from the School of Economics and Business at the University of Ljubljana in a consulting project resulting in a market analysis and a business plan as well as a list of potential partners and financial sources, which led to expressions of interest by potential users of the developed technology in the field of clean environment.

The group also prepared a second **Proof-of-Concept Innovation Fund** call, in the amount of 42,042.42 euros, to fund five JSI research projects and increase their TRLs.

GROUP FOR PROMOTION, EDUCATION AND PROJECT MANAGEMENT

To **encourage researchers** in their entrepreneurial aspirations, the group organizes a competition for the award for innovations with the highest commercial potential. They also organize workshops for young researchers, business model planning and pitch presentations of business-technology propositions. In 2021, six teams applied – four from the JSI and three from more than one PRO. At the 14th International Conference on Technology Transfer, a ceremony for awarding the two best innovations took place. In addition, at the Conference, two WIPO awards were

given: a WIPO Medal for Inventors, recognizing researchers for their impact on society, and a WIPO IP Enterprise Trophy for the company most efficiently utilizing and promoting intellectual property. JSI researchers were also

assisted in presenting their innovations at the ARCA 2021 international fair in Zagreb, winning the silver and two bronze medals.

The group was **informing** the public about its activities through e-newsletters, Facebook, LinkedIn, Twitter and YouTube posts. The group prepared and disseminated lists of Slovenian and EU tenders (12 lists with more than 200 calls) and foreign partner searches (330 initiatives). They disseminated information to TT coordinators weekly, thus efficiently contributing to the submission of new projects with new international partners (30).

Among notable **events**, the group organized the virtual annual Open Day at the JSI and virtual school visits to the JSI (34). It carried out an entrepreneurial education session for young researchers (1 session, 42 participants) and organized the 14th International Technology Transfer Conference with 140 participants. The group also organized the JSI Industry Sprint 2021 with presentations by the JSI researchers as well as companies (42 participants).

The group issued several **publications** – brochure "Modrosti iz inovacijskega okolja v javnih raziskovalnih organizacijah", "Development Opportunities 4" (JSI technologies), "Zaščita in trženje intelektualne lastnine za raziskovalce in podjetja", and "Patents from the Jozef Stefan Institute 1999-2018" (a reissue). The group also coordinated the preparation of a promotional video about the JSI.

- **JSI researchers informed about, and assisted in applying to, domestic and international competitions, winning five awards.**
- **We are members of the European Innovation Council steering board, the advisory group for the Director of the DG R&I of the European Commission, Economic and Societal Impact of Research and Innovation; we lead the working group for establishing the EIC Marketplace for the European Commission; we are national delegates in the CERN Knowledge Transfer Forum. We collaborate with the World Intellectual Property Office (WIPO) within their worldwide international activities. We chair the BioChemTech Group in the Enterprise Europe Network and preside over the Association of Technology Transfer Experts of Slovenia. For the stakeholders in the innovation system, we prepared an overview of the critical points of the transfer of intellectual property from research to industry.**

GROUP FOR CONTRACTUAL COLLABORATION WITH INDUSTRY visits both large and small companies (47), organizes their (virtual) return visits to the JSI (36), organizes sectorial and regional tours of companies to the JSI and collaborates with the other entities from the support environment. This group's members regularly find new topics for cooperation within the development projects amongst companies and researchers (132), prepare technology offers, arrange the signing of non-disclosure agreements, and acquire written consents for further international cooperation with business or technology-research goals. In 2021, 10 international agreements on long-term collaboration were signed. The group also helped sign license and R&D agreements.

The groups mentioned above work closely together. In 2021, the three groups jointly helped close license and research-and-development contracts. The activities of the CTT increased significantly in the area of contracting over the last year, regarding both domestic and international contracts.

GROUP FOR SUPPORTING PROJECT PROPOSALS AND EXECUTION

Since the establishment of the Center for Technology and Innovation Transfer on 1 January 2011, this group has, along with its partners, submitted a number of successful applications to various national and European tenders. Group members are evaluators of Slovenian and international project applications. They work in different committees

for the preparation of guidelines and calls at different levels. For example, they participated in the working group of the European Commission, which set the guidelines for the operation of the European Innovation Council. The group was later even named the EIC National Champion. The group is a member of the European Enterprise Network and Vision 2020, which provide important tools for its work. The group has gained important and vast experience in the field of project preparation and implementation, on the basis of which its experts can competently advise and help the researchers at the Institute.

The group offers assistance to interested JSI departments in **preparing project applications** by updating the **call search database** on a monthly basis (1600 calls in 2021); it provides assistance with individual **tender schemes**, **interpretation of tenders**, the **search for project partners** (30) and the **preparation of individual sections** of project applications (17) (e.g., management, communication & dissemination, impact). JSI researchers can also contact the group experts if they need help in preparing **legal documents** related to project applications, e.g., NDA between partners, and

Figure 3: Awards for JSI Researchers from the ARCA International Exhibition of Inventions 2021 in Zagreb, Croatia

in preparing consortium agreements, especially in reviewing **background IP** and foreseeable, i.e., **foreground IP**, as well as in giving advice on the management of IP for an annex to a consortium agreement. They also advise on the **legal aspects of European research programs** (e.g., state aid, intellectual property, open access, FAIR, open science). They offer assistance to interested departments in the implementation of projects, especially in the area of management and impact, and in the preparation of deliverables from these sections.

GROUP FOR INNOVATION RESEARCH

Experts from this group operate as **evaluators and external experts** in Slovenia and within the European Commission, as well as different respectable international institutions (EC ERC, EUREKA, RRI). They were recognized by the JRC as one of the most propulsive technology transfer offices in the EU and were included into the **TTO Circle**, a group of PROs most active in the field of knowledge and technology transfer (including the institutes Max Planck, Weitzman, Fraunhofer, VITO and VTT). They collaborate with the **United Nations**, as a member of the 10-member Group for Support of the Technology Facilitation Mechanism (10MG TFM), and with the **World Intellectual Property Office** (WIPO) in the context of its international worldwide activities. The group is a member of the Expert Group **DG Research & Innovation in the European Innovation Council**. In 2021 the group continued its membership within the Materials and ICT **Sector Groups within the Enterprise Europe Network**. It holds the **chairmanship** of the BioChemTech Group, participates in the steering board of the European Innovation Council, and the HL Advisory Group of the Director of DG R&I Economic and Social Impact of Research and Innovation. The group presides over the Association of Professionals for Technology Transfer of Slovenia, as well as the Committee for Spin-Out Creation at the Jožef Stefan Institute. In 2021, within the CRP (ARRS) project, the group identified key critical points in the transfer of intellectual property (IL) from research organizations to industry to help relevant stakeholders in the innovation ecosystem, which will be beneficial to further IL evaluation processes as the basis for proposing a long-term sustainable state-aid model, promoting cooperation between science and industry.

Organization of Conferences, Congresses and Meetings

1. 14. International Technology Transfer Conference - 14.ITTC; (live + virtual), 7.-8.10.2021
2. Young Hopes 2021 – Entrepreneurial and innovation workshop for young researchers; (virtual), 23.4.2021
3. Hackathon "Researchers and Companies Hand-in-hand for our Better Tomorrow" - (virtual), 9.7.2021
4. JSI Industry Sprint 2021: short presentations by JSI researchers and company representatives for collaboration opportunities – (virtual), 16.9.2021
5. Cooperation meeting Cracow University of Technology – Jožef Stefan Institute – (virtual), 9.12.2021

INTERNATIONAL PROJECTS

1. K7, CTT - ID Creations; Rights and Obligations regarding the Development, Use and Commercialization of Hydrothermally Synthetized TiO2 Coatings in Metal Orthopaedic and Dental Implants
   Dr. Špela Stres
   Id Creations Oy
2. COSME-EEN-SGA4 - EEN Slovenia 4; EEN Slovenia Services in Support of Business and Innovation in Slovenia
   Dr. Špela Stres
   European Commission
3. H2020 - KET4CleanProduction; Pan-European Access for man.SME on tech. services for clean production through a Network of premier KET Technology Centres with one stop shop access incl. EEN and discourse with policy makers on RI3
   Dr. Špela Stres
   European Commission
4. H2020 - AMULET; Advanced Materials and Manufacturing Technologies united for LightwEight

Dr. Špela Stres
European Commission
5. H2020 - We4SMESLO 5; Enhancing Innovation Management Capacity in Slovenian SMEs by EEN Slovenia
   Dr. Špela Stres
   European Commission

R&D GRANTS AND CONTRACTS

1. Evaluation of IP as a basis for proposing a long-term sustainable state aid model to promote science-business cooperation
   Dr. Špela Stres
2. The consortium for technology transfer from the PRO to the economy
   Dr. Špela Stres
   Ministry of Education, Science and Sport
3. JSI Share of License Revenues related to Exploitation of Inventions - Abroad (JSI License Revenue Share - Abroad)
   Dr. Špela Stres

VISITORS FROM ABROAD

1. Bojan Čudić, Enterprise Europe Network BiH, Bosnia and Herzegovina, 11.6.2021
2. Alexandre Massart, Vesna Capital LLC, London, UK, 15.6.2021
3. Magdalena Wencka, Institute of Molecular Physics, Polish Academy of Sciences, Poznan, Poland, 26.7.2021
4. Jernej Dvoršak, BABEG Kärntner Betriebsansiedlungs- und Beteiligungsgesellschaft mbH, Klagenfurt, Austria, 2.9.2021
5. Jacek Kacz, Cracow University of Technology / Politechnika Krakowska, Krakow, Poland, 3.9.2021
6. Alexandre Massart, Vesna Capital LLC, London, UK, 7.9.2021
7. Jana Kolar, European Strategy Forum for Research Infrastructures (ESFRI), Trieste, Italy, 10.9.2021
8. Toshiyasu Ichioka, RIKEN Europe Office, Brussels, Belgium, 25.10.2021
9. Do-won Lee, Ki-young Ko and Jun-ho Ko, Korea Invention Promotion Association (KIPA), Seoul, South Korea, 8.11.2021

STAFF

Researchers
1. Dr. Marijan Leban
2. Dr. Duško Odić
3. Dr. Levin Pal
4. **Dr. Špela Stres, Head**

Postgraduate
5. Robert Blatnik, M. Sc.

Technical officers
6. Tomaž Justin, B. Sc., MBA

7. Tomaž Lutman, B. Sc.
8. Urška Mrgole, B. Sc.
9. France Podobnik, B. Sc.
10. Marjeta Trobec, M. Sc.

Technical and administrative staff
11. *Gregor Jus, B. Sc., left 01.07.21*
12. Matej Mrak, B. Sc.
13. *Miha Pitako, B. Sc., left 01.07.21*
14. Robert Premk, B. Sc.

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4. Špela Stres, Mirica Karlovits, Vojka Žunič, Robert Blatnik, Tomaž Lutman, Marjeta Trobec, "Proof of Concept sklad: nujen finančni instrument", In: *Modrosti iz inovacijskega podpornega okolja v javnih raziskovalnih organizacijah za upravljavce inovacijskega sistema*, Institut "Jožef Stefan", Fakulteta za informacijske študije Novo mesto, Kemijski inštitut, Kmetijski inštitut Slovenije, Nacionalni inštitut za biologijo, Univerza na Primorskem, 2021, 74-93.
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1. Špela Stres *et al.* (17 authors), *Modrosti iz inovacijskega podpornega okolja v javnih raziskovalnih organizacijah za upravljavce inovacijskega sistema*, Institut "Jožef Stefan", Fakulteta za informacijske študije Novo mesto, Kemijski inštitut, Kmetijski inštitut Slovenije, Nacionalni inštitut za biologijo, Univerza na Primorskem, 2021.

CENTER FOR SMART CITIES AND COMMUNITIES

CSC&C

The Center for Smart Cities and Communities (C SC&C) was established at the beginning of 2017. On 1 January 2019, Dr. Nevenka Cukjati, Ph. D., took over the management of the center.

The main task of the center is to coordinate and operate the Strategic Development and Innovation Partnership of Smart Cities and Communities (SRIP SC&C). In addition, the center also promotes cross-sectoral cooperation within the Jožef Stefan Institute, thus supporting the partnership in the field of state-of-the-art technologies and, at the same time, actively participating in the creation of national R&D policies for the coming years.

Head:
Dr. Nevenka Cukjati

Strategic Development and Innovation Partnership of Smart Cities and Communities

Strategic Development and Innovation Partnership of Smart Cities and Communities (SRIP SC&C) is a form of partnership, in which stakeholders have joined forces in developing and selling solutions to raise the quality of life in cities of the future.

The aims of SRIP SC&C are to connect companies and research institutions in a particular field into value chains, set **priorities for development investments** and coordinate R&D activities. We are building a **good support environment** for sharing knowledge and experiences in the form of workshops, seminars and joint events; we offer access to test environments, laboratories, databases; and we provide assistance in market analyses, human-resource development, intellectual-property protection and internationalization.

We want to approach smaller towns in Central and Eastern Europe with innovative solutions as we consider Slovenia a very suitable reference country for various "smart urban" solutions, which could be implemented in other parts of Central and Eastern Europe.

SRIP SC&C was formally constituted at the Assembly on 23 March 2017, and it currently includes 119 Companies and Research Institutions from all over Slovenia (Table 1).

Key areas and technologies

Strategic Development and Innovation Partnership of Smart Cities and Communities covers several research areas as well as ICT horizontal key enabling technologies (Figure 1).

SRIP SC&C creates and supports **business and research synergies** in Smart Cities, aids the development of new products, services and technologies. We help companies enter the global market by focusing on niche areas, with the aim of making Slovenian companies an important European provider of such solutions.

The partnership includes the contents of the current financial perspective Europe 2021–2027, the Mission Area of Carbon-Neutral Cities and the guidelines of the GREEN DEAL document. Through the mission's financial mechanism, the European Commission identified the importance of carbon-neutral smart cities as one of the five key areas.

Organization type	Micro	Small	Medium	Large	Faculty / Institution	Municipality / Association	Total in SRIP SC&C
Number of organizations in SRIP SC&C	38	29	14	11	19	8	119
KEY SEGMENTS							
HEALTH	19	11	7	2	14	4	
ENERGY AND UTILITIES	17	14	9	9	12	6	
MOBILITY, TRANSPORT AND LOGISTICS	22	19	7	6	11	5	
SAFETY	18	9	2	3	10	3	
URBAN LIFE QUALITY	18	10	4	1	11	5	
SMART CITY ECOSYSTEM	25	17	8	4	13	5	
TEHNOLOGIES							
INTERNET OF THINGS (IoT)	23	14	9	5	12	4	
INTERNET OF SERVICE (IoS)	22	15	7	7	10	3	
GIS-T	9	9	4	1	10	2	
HPC AND BIG DATA	12	10	4	4	11	2	
CYBER SECURITY	12	8	3	3	11	1	
DIGITAL TRANSFORMATION	22	18	7	5	13	5	

Table 1: Distribution of SRIP SC&C members

Figure 1: Key areas and technologies

Partnership goals:
- creating and supporting synergies between companies, research and development;
- creating a connection between the state and members of SRIP SC&C: active participation in policy creation and formulation of new financial perspectives 2021–2027 and further until 2030: Slovenian Industrial Policy (SIP), Development-Research Strategy of Slovenia, Artificial Intelligence Strategy, Smart Specialization Strategy (SPS);
- promoting its members and their products and services;
- providing direct information to the SRIP SC&C members;
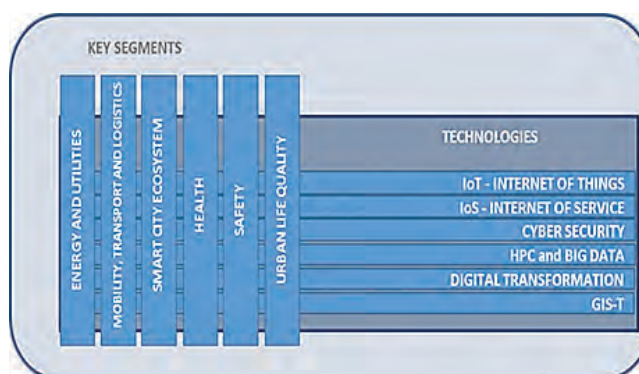- improving the quality of life in cities and communities: collaboration with municipalities, cities.

Activities within the organizational structure of SRIP SC&C

On 10 June 2021, at the 4th Regular Assembly of SRIP SC&C members, we approved the SRIP SC&C Annual Report for 2020 and SRIP SC&C Financial Report for 2020; we also presented the reports of the Steering Committee and the report of the SRIP SC&C Program Council. We became acquainted with the proposed indicators for monitoring the performance of SRIP in the period 2020–2022. These indicators, proposed by the Government Office for Development and European Cohesion Policy (SVRK), were properly adjusted for the assessment of the operation of SRIP SC&C. We also got acquainted with the renewal of the Slovenian Smart Specialization Strategy – S4, defining the period of the new financial perspective 2021–2027.

Renewal of the Slovenian Smart Specialization Strategy – S4

We participated in the process of renewing the Slovenian Smart Specialization Strategy – S4. At the introductory workshops on 26 March 2021, SVRK presented the planned process of renovation of S4 for the period 2021–2027 and the relevant professional and programme foundations of the Ministry of Education, Science and Sport (MIZŠ), Ministry of Economic Development and Technology (MGRT), Ministry of Labour, Family, Social Affairs and Equal Opportunities (MDDSZEM) and Government Office for Development and European Cohesion Policy (SVRK).

This was followed by nine domain or field web workshops, at which individual SRIPs together with SVRK presented concrete proposals of the focus areas and product directions, identified in the previous phases of the entrepreneurial research.

Free promotional interactive events for the members of SRIP SC&C

We were the organizers of the online Smart Cities 2021 Conference, which took place on 16 September 2021. At the conference we discussed climate-neutral cities. Europe is committed to achieving the 2030 goal of climate neutrality and ensuring environmental sustainability for a better future for all people, both in Europe and beyond. Examples of good practices of companies in the Slovenian municipalities and the trends and opportunities used in Europe in terms of reducing the carbon footprint were presented. Representatives of the economy, research organizations, municipalities, non-governmental organizations and the state administration met at four round tables.

In the Slovenian Digital Center, BTC City Ljubljana, we participated in the event Public and Private Security Week, which took place during 11–14 October 2021. Slovenian companies, research organizations, ministries, professional users and other organizations and individuals presented their products, solutions, projects and views in the field of public and private security. The event consolidated the ecosystem of the stakeholders in this field, established in the Strategic Innovation Partnership of Smart Cities and Communities and within the 5GSafety project. The members of SRIP SC&C Vertical Security prepared a digital environment DIGITAL EXPO - SAFETY for the event, providing a comprehensive hybrid approach to the presentation of solutions, projects, services and other ideas and cooperations.

In the Slovenian Digital Center, BTC City Ljubljana, and remotely, we participated in the Month of Industry 4.0 and Robotics. The event ran from 27 November to 22 December 2021 and included more than 30 events aimed at high-school students, college students and young researchers. Young entrepreneurs, companies or their representatives from Slovenia and Europe were also invited. As part of the event, we organized the Congress: How can Industry 4.0 support development of Smart Cities, which took place on 9 December 2021. The event connected smart cities and communities with Industry 4.0 and Robotics.

As part of the **promotion and internationalization**, a short film was prepared at the initiative of SPIRIT Slovenia for EXPO DUBAI 2020, within the SRIP SC&C operation, presenting available smart solutions and products from Slovenian cities. The field of Smart Cities and Communities was presented in the period from 31 October to 6 November 2021.

Online platform: Smart City

In cooperation with the expert group from the University of Ljubljana, Faculty of Computer and Information Science (UL FRI), we prepared SRIP SC&C open source web platforms: Technology Gameroom and Solution Market. In the Technology Playroom, you can get to know and test different technologies and platforms (games) for the development of innovative solutions in the field of smart cities and communities. However, you can share and promote your solutions in a common digital marketplace.

SI4CARE project

The SI4CARE project seeks to provide the elderly population in the ADRION regions with health care. The main purpose of the project is to combine strategies and action plans in individual countries (Slovenia, Italy, Croatia, Bosnia and Herzegovina, Greece, Montenegro, Serbia) and use them in practice to help the elderly, especially in remote places.

Due to the lack of space in nursing homes and the desire of the elderly to stay in their own environment as long as possible, solutions are being created that make it easier to live in a home environment. In Slovenia, we would like to bring together all the solutions and connect with the stakeholders from other countries through SI4CARE.

The leading partner in the project is the University of Ljubljana, with eight partners from seven countries. The Departments of Computer Systems (E7) and Intelligent Systems (E9) are participating in the SI4CARE project: Social innovations for the integrated care of the aging population in the ADRION regions. The project is co-financed by the Interreg ADRION programme (European Regional Development Fund - ERDF) with just over 2 million euros.

In 2021 two SI4CARE meetings took place. One was held on 15–16 July 2021 in Split, Croatia, where the topics discussed included the ongoing activities, an analysis of the situation and the activities planned for the future. The second SI4CARE meeting was held in Vrnjačka Banja (Serbia) on 21–22 October 2021, giving a presentation of the current situation and challenges regarding the elderly in Serbia. The biggest challenge in the region is a lack of integrated long-term care services.

In Novo mesto, on 8 September 2021, the City of Novo mesto, together with the University of Ljubljana, organized a conference entitled Slovenia's Responses to the Challenge of an Aging Society where the issue of an aging society was presented.

In recent years, the Jožef Stefan Institute has developed several technologies that have the potential to be used in the field of long-term care. The EkoSMART project, in which some members of SRIP SC&C also participated, was very successful. The technologies that have been developed are aimed at healthcare professionals as well as caregivers–family helpers – and end users.

Examples of solutions for various applications include: OPKP diet planning, serious games for the telerehabilitation PD manager, or sensors for monitoring and remote assistance.

HeartMan is an application planned as a pilot within the SI4CARE project, which will be simplified for this purpose and thus accessible to as many patients as possible.

It was developed for the Horizon 2020 project and coordinated by the JSI. It provides individual patients with a tool for medication based on measured body parameters, an adjustable exercise program, monitoring of and advice on diet, psychological support using cognitive-behavioural techniques and mindfulness, etc.

The results of the project are regularly published and updated on social networks.

New Financial Perspective: EU missions

EU missions represent a new way of tackling important societal challenges. Horizon Europe (2021–2027) identified the following key missions: fighting cancer, adapting to climate change, living in greener cities, caring for soil health, for healthy food, people, nature and climate, protecting the oceans. These missions will go beyond research and innovation, promoting innovation in different sectors to provide effective solutions. They will also play a key role in pursuing EU priorities, e.g., the European Green Agreement. The emphasis is on a more efficient use of resources through the transition to a clean, circular economy, restoration of biodiversity and reduction of pollution. The European Green Agreement aims to make the EU the first carbon-neutral continent by 2050.

The Mission for Climate Neutrality and Smart Cities will support, promote and represent 100 European cities in their transformation to climate neutrality by 2030 and turn them into centres of experimentation and innovation for all cities. The mission aims to promote a fair transition to improve people's health and well-being and provide many additional benefits of the transition, such as better air quality, job creation and a healthier lifestyle. At the heart of this mission will be people living in cities. In addition to the involvement of the population, the involvement of companies in need of the support for the transition to low-carbon operations is also important.

SRIP SC&C, which includes 119 organizations and has relevant information and resources, is involved in the activities related to the 100 Climate Neutral Cities by 2030 initiative under the Mission's financial instrument. As part of the ZMOS activities, SRIP SC&C will take on the role of a one-stop shop for the implementation of climate-action plans and a social-innovation hub to support international exchange of experience in implementing climate plans and can serve as the reference point for preparing Strategies and Action Plans, which are a condition for the cooperation, in line with the guidelines of the Green Deal call.

Some solutions created by the SRIP SC&C members that can be included in the programme are as follows: establishing a system for collecting, processing and interpreting data on climatic and microclimatic conditions in a city; introducing the measures for energy efficiency of buildings; ensuring adequate greening of cities for adequate ventilation of cities; providing sustainable and carbon-neutral energy and other supplies; introducing clean and sustainable energy-production systems and introducing smart-transport systems for urban supply that will reduce emissions and provide the necessary supply.

R&D GRANTS AND CONTRACTS

1. Social Innovation for Integrated health CARE of ageing population in ADRION Regions-SI4CARE
    Dr. Nevenka Cukjati
    The Emillia-Romagna Region
2. Support for Strategic Research and Innovation Partnerships (SRIP) in priority areas of Smart Specialization

Dr. Nevenka Cukjati
Ministry of Economic Development and Technology
3. Support for Strategic Research and Innovation Partnerships (SRIP) and Priority Areas of Smart Specialization (SRIP PMiS)
    Dr. Nevenka Cukjati

STAFF

Technical officer
1. Dr. Nevenka Cukjati, Head
Technical and administrative staff
2. *Petra Hauschild, B. Sc., 21.04.21, transferred to Department CTOP*

3. Mojca Kristl, B. Sc.
4. Jan Kunc, B. Sc.

CENTER FACTORIES OF THE FUTURE

CFoF

The center was established in early 2017. The main task of the center is to coordinate and realise the Strategic Development and Innovation Partnership of Factories of the Future (SRIP FoF). In addition, the center also encourages cross-sectoral cooperation within the Jožef Stefan Institute, thereby contributing to the support of the latest technology partnership and, at the same time, actively participating in the development of R&D policies for the coming years.

What does the Factories of the Future Strategic Development Innovation Partnership offer?

The SRIP Factories of the Future (SRIP FoF) strategy is to gather and integrate Slovenian research and innovation knowledge and experience from the industrial and academic spheres and highlight the priority breakthroughs of new products, technologies and services for Factories of the Future. We have established a supportive environment with expert services for industry and research organizations, with an emphasis on developing new cutting-edge technologies that combine and build on the existing Slovenian research and innovation achievements.

The key functions of the strategic long-term interconnectivity are the definition and upgrade of the strategic action plan for Factories of the Future, activities in the scope of the development of joint services, internationalization, development of human resources, representation of joint interests to the state, etc. Part of the services will be done in cooperation with other institutions.

SRIP FoF **creates and supports** business and research synergies in the area of smart factories for new products, services and technologies, and helps businesses enter the global market by focusing on niche areas. The 95 members of SRIP FoF come from various companies, associations or institutions from Slovenia. The operation of SRIP FoF focuses on a greater integration of knowledge and joint presentation of stakeholders in domestic and international markets. The primary goals are to increase the share of high-tech industrial products in the exports and increase the added value of the Slovenian industry.

Head:
Rudi Panjtar , B. Sc.

Key areas of activities

The SRIP Factories of the Future includes eight areas (verticals) and horizontal networks, interconnected by the key technologies (Figure 1).

By effectively directing R&D and introducing knowledge and technologies that enable the production of better-quality products, reducing energy and raw materials, reducing environmental pollution, improving human involvement, etc., SRIP FoF also indirectly contributes to accelerating the transition to a low-energy, energy-efficient economy and greenhouse-gas emissions, thus intensively promoting the transition to a low-carbon society and a circular economy. The essence of the concept of factories of the future is mainly reflected in a greater potential for the reuse of raw materials, made possible by a more flexible and optimally managed production.

In the field of **internationalization**, we were actively involved in the economic diplomacy at the Ministry of Foreign Affairs and the SPIRIT Agency. In the preparatory period of Slovenia's Presidency of the Council of the European Union, we highlighted some topics in our field at the events held in the Digital Center of Slovenia in the BTC, organised under the common slogan Digital Center of Slovenia – Technology for People, between 27 November and 22 December 2021, and marked by Industry 4.0 and Robotics. At the beginning of the presidency, we provided an e-brochure of examples of good practices of the circular/digital economy in Slovenia, presenting the

Figure 1: Scheme of SRIP FoF domains

Circular 4.0 project and SRIP FoF JSI, which was forwarded to the prime ministers of the EU Member States, the European Parliament, the President of the European Commission and other representative organizations. SRIP FoF members also participated in other accompanying events during Slovenia's Presidency of the EU Council. At the end of Slovenia's Presidency, we published a brochure entitled Industry 4.0 and Robotics. We participated in the events of the World Manufacturing Forum and EUSAIR at the end of October 2021 and prepared the WMF Report 2021 "Digitally Enabled Circular Manufacturing". We actively participated in the activities of the EFFRA (European Federation for Factories of the Future Research Association), where we became members of the board of directors of the organization and monitored the design of the Made in Europe programme. We joined the start-up activities for
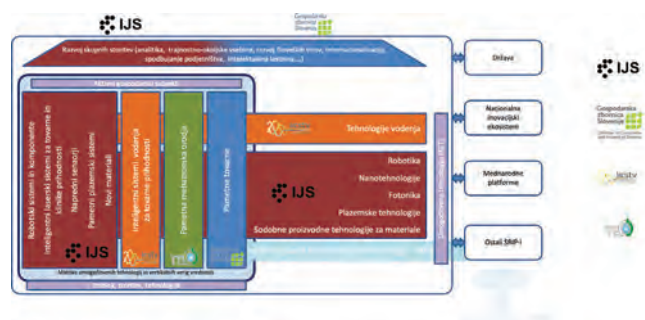
the installation of the Gaia X Slovenian junction organized by DIH Slovenia. We participated in the events organized by the Slovenian Business & Research Association (SBRA) and Ministry of Education, Science and Sport (MIZŠ) in the field of new funding programmes (European Space Agency (ESA) – Space Programme and European Defence Fund). We built the international recognition of SRIP and new partnerships, strengthening the international reputation of SRIP FoF, the Jožef Stefan Institute and other SRIP FoF beneficiaries.

SRIP FoF was presented at the LAC (Latin America Countries) Conference, in cooperation with the Ministry of Education, Science and Sport, on 22 April 2021; SRIP FoF participated in the Bled Strategic Forum on 12 May 2021, and the EUSAIR Forum on 26 February 2021, AFIL Lombardia, organized by the Ministry of Foreign Affairs.

To expand and consolidate its activities in the field of innovation at home and abroad, the JSI, as the coordinator of SRIP FoF, is actively involved in various European initiatives. One of these is the European Institute of Innovation and Technology (EIT), which enables innovators and entrepreneurs to develop solutions to create growth and jobs.

Thus, SRIP FoF has been actively present in the field of manufacturing through the JSI since the beginning of the creation of the **EIT Manufacturing** – EITM community (https://eitmanufacturing.eu/), and in 2021 it became its full member. To support the implementation of the EITM Programme at the JSI, the institute was organized internally. In its development phase, it sent an informative invitation to all the departments and centres at the JSI; seven departments responded, all of which are members of the SRIP FoF and the Factories of the Future Center. In doing so, the rules for joining the EITM were concluded and adopted. Based on this, the JSI as a member and coordinator of SRIP FoF, worked in the EITM innovation ecosystem, participated in the development of the key topics in production technologies and processes, participated in decision-making on global issues, exchanged industrial experiences at the European level, defined the key requirements and applied to calls for EITM projects. As a member, the JSI was also able to invite external partners who are not members of the EITM to participate in the projects, but of course the SRIP FoF members had priority.

The year 2021 was marked by the 3rd phase of the SRIP ToP project, when we further intensified our activities, though they were still affected by the COVID 19 epidemic and the related measures both at home and abroad. In implementing the activities, we followed the action plan for the **3rd phase of the SRIP operation**, met with the coordinators of individual vertical value chains and horizontal networks and encouraged them to connect with the members in preparing joint projects and events of interest to the members, research sector and industry. We continued to cooperate with other SRIPs, the key ministries that are important for our work (MGRT, MIZŠ) and the Government Office for Development and Cohesion Policy (SVRK). We established contacts with new teams in key ministries and actively participated in the discussion and preparation of the operational programmes for the next financial period.

In cooperation with SVRK we made changes to the process of entrepreneurial discovery in certain product and development areas, which will be included in the **renewed strategy of smart specialization for the period 2021–2027**. We highlighted the **importance and inclusion of key enabling technologies**, the development and financing of which are crucial for the success of the entire Slovenian smart specialization as well as for the JSI.

We conducted SRIP ToP presentations at various events and presented SRIP ToP and our activities at various meetings at home and abroad. We were active in collecting and preparing **news for the members**, and our website was well visited as it is a hub of the news about the technology and our activities. In combination with social networks, an increasing number of followers acquaint themselves with our activities. We published weekly news that was received well by the readers.

To encourage organizations to join SRIP FoF, we conducted several presentations of SRIP FoF in 2021. Among the most resounding ones was also the event called Transformation of the Automotive Industry, prepared in collaboration with Unior, a member of SRIP FoF. At the session of the Commission for Science, Education and Culture at the National Council, we presented the **National Demo Center** project. Together with the Chamber of Commerce and Industry, we co-organized the event Challenges and Opportunities for Interinstitutional Cooperation in the Field of Human Resources Development.

We would like to emphasize the events organized during the Slovenian Presidency of the European Council, which took place in the Digital Center of Slovenia in the BTC under the common name Digital Center of Slovenia – Technology for People. December events in the Digital Center of Slovenia took place between 27 November and 22 December 2021 and were dedicated to **Industry 4.0 and Robotics**. The rich programme of December was intended for professionals and the general public, created under the auspices of SRIP Factories of the Future (SRIP FoF) in cooperation with MGRT, Spirit, BTC and DIH Slovenia as well as with several JSI departments, Center for Technology Transfer and Innovation at JSI, and other partners from Slovenia and abroad. The Digital Center hosted free robotics and fun programming workshops for children and other groups interested in robots. Experiments and the abilities of robots to work with humans were presented, showing the solutions that make it easier for companies and organizations to produce and operate, thus consolidating Slovenia's Digital Center in December as a crossroads of Slovenian development and economic progress in Industry 4.0 and robotics.

We have maintained the connection we developed with **KOC-FOF** in the past, giving our members access to the workshops and conferences organized by KOC-FoF.

In 2021, **11 new members** joined SRIP FoF: BeeIN, d.o.o.; CADCAM LAB, Company for computing, design, production, representation and engineering, d.o.o.; Gram Commerce d.o.o.; IB-CADDY information technologies d.o.o.; PINA Cultural and Educational Association, Associazione Culturale Ed Educativa Pina; Result d.o.o., SAŠA incubator, company for entrepreneurial and business consulting, d.o.o.; Slovenian Institute for Quality and Metrology, Ljubljana; SIST – Slovenian Institute for Standardization; Termo Shop d.o.o.; Association for Engineering at the Chamber of Commerce and Industry.

Throughout the year we actively participated in the **QU4LITY** project under the scope of the H2020 initiative, which is expected to demonstrate, in a realistic, measurable and replicable way, an open, certifiable, highly standardised, SME-friendly and transformative shared data-driven ZDM (zero-defect manufacturing) product and a service model for Factory 4.0. Within this project, the SRIP FoF is working with the JSI Department for Automation, Biocybernetics and Robotics as one of the leading partners in Work Package 8; it is also collaborating with a consortium of partners to design and implement a virtualized platform, which will include a project marketplace where all the ZDM equipment will be listed and marketed, and a digital innovation hub, which will offer innovation management services. SRIP FoF was involved in the coordination of the virtual platform implementation, which is expected to be publicly accessible in 2022.

In December 2018 we joined the Interreg Mediterranean project **Panoramed** as a co-leader in the field of innovation. In 2022 we continued with the planned work commitments. We regularly met with Slovenian representatives of the two selected strategic projects in the field of Innovation. Project BlueBioMed promotes the transformation of the development and improvement of sustainable goals in the field of innovation for blue bio-technologies in the Mediterranean. The project focuses on the development of innovation policies in correlation with the transnational governance programmes of the Mediterranean Region. Project B-Blue, however, is based on connecting communities of the Mediterranean. These are bringing together the key figures from the blue bio-technologies with the goal of increasing their capacities and coordination as means of maximising the innovation potential through common transnational initiatives. They are planning to include the organizations from the Southern Mediterranean as well. Both strategic projects work alongside one another in pursuit of better results. By presenting the past activities and participating in the planning of future work, we were involved in all project meetings that took place online due to the epidemic during this period. In 2021, in cooperation with the leaders of the strategic projects in the field of innovation, we prepared questionnaires for the follow-up, collected data and prepared the first and second follow-up reports. We also participated in several international online events in the field of blue bio-technologies, as well as events of the strategic projects within the framework of Innovations, and presented our work so far at two events. We are also in regular contact with the SVRK representative, who is engaged in the Panoramed Project.

At the beginning of 2020, the Center for FoF launched the project *Digital technologies as an incentive for the transition to a circular economy by small and medium-sized enterprises in the Alps – **CIRCULAR 4.0**. The project is funded by the Interreg Alpine Space programme. The aim of the CIRCULAR 4.0 project is to accelerate the transition of small and medium-sized enterprises from the Alpine Region from a linear to a circular business system through digitalization and Industry 4.0.

As part of the second work package aimed at establishing circularity and digital assessment tools and a training programme for companies and support organizations, the Center for FoF prepared and tested a training programme for intermediary organizations in 2021, in cooperation with two JSI research departments, an external contractor, project partners and test companies from the whole Alpine Region. The Center was involved in the development of new tools and review of the existing tools for assessing the circularity and the degree of digitalization of companies, and with the help of the SRIP FoF members, also in testing the applicability of the proposed tools. The total value of the project is €2,560,692. Fifteen project partners from five Alpine countries are participating – Austria, Italy, France, Slovenia, Germany: Amt der Salzburger Landesregirung, Associazione Fabbrica intelligente Lombardia, Austria Wirtschaftsservice Gesellschaft, Auvergne-Rhône-Alpes Enterprises, Bundesministerium fur Digitalisirung und Wirtschaftsstandort, BWCON, Camera di Commercio Industria Artigianato e Agricoltura di Venezia Rovigo, Chambre de Commerce et d ' Indsutrie du Var.

Grant Agreement number: 970904 – MANAGING DIGITAL INTELLECTUAL PROPERTY IN MANUFACTURING SMES DIGITALIZATION PROCESSES (**Go-DIP**)

In 2021 we were successful with our proposal for a new project within the Horizon Innosup programme for small and medium-sized enterprises in the field of **digital data management in enterprises**. The result of the project will be a handbook of the tools for managing digital data in enterprises and examples of business practices from three innovation systems. The duration of the project is 13 months. The cooperating partners are HIT – Hub

Innovazione Trentino Fondazione, Italy, and Haute Ecole Specialisee de Suisse Occidentale / HES-SO- INNOSQUARE Freiburg-Switzerland.

We also completed work on the **HIA (High Impact Action)** project, funded by the EC. After the completion of the project, it is planned to prepare a specification for the establishment of a comprehensive smart factory platform, which will be the basis for the establishment of a national demo center, integrating Slovenian knowledge and demonstrating a practical approach to the vision of the future.

INTERNATIONAL PROJECTS

1. H2020 - QU4LITY; Digital Reality in Zero Defect Manufacturing
   Asst. Prof. Igor Kovač
   European Commission
2. H2020 - Go-DIP; Managing Digital Intellectual Property in Manufactoring SMEs Digitalization Processes
   Asst. Prof. Igor Kovač
   European Commission

R&D GRANTS AND CONTRACTS

1. MED Governance Platform
   Asst. Prof. Igor Kovač
   Government Office for Development and European Cohesion Policy
2. Circular 4.0: Digital technologies as enabler to foster the transition to the circular economy bythe SME in the Alpine Space area
   Asst. Prof. Igor Kovač
   Government Office of the Land of Salzburg
3. Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF)
   Asst. Prof. Igor Kovač
   Ministry of Economic Development and Technology

STAFF

Researcher
1. Asst. Prof. Igor Kovač
Technical officers
2. Živa Antauer, B. Sc.
3. Petra Lavtar, B. Sc.
4. Bojana Omersel Weeks, B. Sc.

5. **Rudi Panjtar, B. Sc., Head**
Technical and administrative staff
6. *Matic Eržen, B. Sc., left 19.03.21*
7. Petra Hauschild, B. Sc.
8. Tina Mrak Maržić, B. Sc.
9. Nataša Vertot Rakun, B. Sc.

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1. Timotej Gašpar, Igor Kovač, Aleš Ude, "Optimal layout and reconfiguration of a fixturing system constructed from passive Stewart platforms", *Journal of manufacturing systems*, 2021, **60**, 226-238.

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1. Primož Radanovič, Jaka Jereb, Igor Kovač, Aleš Ude, "Design of a modular robotic workcell platform enabled by plug & produce connectors", In: *ICAR 2021, 20th International Conference on Advanced Robotics, 7-10 December 2021, Ljubljana, Slovenija*, Proceedings, IEEE, 2021, 304-309.