Annual Report 2020

Jožef Stefan Institute, Ljubljana, Slovenia

JSI REPORT P-334
ANNUAL REPORT
2021

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Publisher: Jožef Stefan Institute, Jamova cesta 39, Ljubljana, Slovenia

http://www.ijs.si

Editors: Dr. Luka Šušteršič, Marjan Verč, M. Sc.

Language adviser: Asst. Prof. Paul John McGuiness

ISSN 1318-7392

Photography: Marjan Verč, M. Sc., Marjan Smerke and departmental archives

Layout: Marjan Verč, M. Sc.

Ljubljana, 2021

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INTRODUCTION

The year 2020 was marked by the Covid-19 pandemic. In just a few short months we went from a comfortable position and an optimistic vision of the future, to the kind of state of emergency that most of us only knew from history textbooks. It was as if suddenly, all the problems hit us at once: from the climate crisis, the crisis of social systems, unbridled technological development that our social intelligence is not able to follow, to the inability to solve the problems of migration while closing in on self-sufficient social environments. The emergence of the SARS-CoV2 virus seems to have highlighted all these problems and made us realize that we are not superior to nature. This realization was very hard to take, and it is not over yet.

Science has tried, and is still doing its best, to limit the consequences of the pandemic. It has proved how indispensable the role of science is in modern societies. When we researchers suddenly found ourselves working from home in March, probably most of us were overwhelmed by feelings of uselessness and helplessness, at our inability to act and become involved in resolving the crisis. However, many of our colleagues quickly became aware and offered their expertise in various fields to the public, from testing protective equipment, to searching for new medicines, to modelling the development of the pandemic. In times of seemingly insurmountable obstacles, it has become really clear how knowledge, diligence, dedication, trust in verifiable facts and cooperation on a global scale are the virtues of scientific engagement that can lead us out of this crisis. Unfortunately, science, even more than ever before, has encountered modern obstacles in the form of online confusion, commentators who claim to know it all, and sensationalism. At our Institute, we are used to such challenges. They encourage us even more to fulfil our mission, part of which is, and will remain, to consider the scientific facts rather than shamanism, helping society to get back on its feet and regain the sense of security that drove it forwards in the times before the pandemic.

Prof. Jadran Lenarčič hands over to Prof. Boštjan Zalar, the new JSI director, on 1 December 2020.

It is gratifying to note that our core activity has not suffered because of the health crisis. Thus, in 2020 the number of scientific publications increased to 1,376, there were 20 scientific and professional monographs published, and 17 patents were granted. According to the Web of Science database, the publications of our colleagues were cited more than 46,000 times. Thirty-nine doctorates have been awarded. The situation in Slovenian science is noticeably improving, which is reflected in the JSI's revenue growth, the number of employees and the number of young researchers. In international cooperation, the Institute's involvement in the European Research Area is particularly strong, which is reflected in the growth of revenues from its own activities in the European market. Finally, in 2020 three European Research Council (ERC) grants were awarded to staff at the JSI.

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

2003

- Jožef Stefan International Postgraduate School established

2004

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

2007

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

2015

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

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. Boris Frlec, 1975–1984
Prof. Tomaž Kalin, 1984–1992
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 31 March 2020 [2] since 1 April 2020

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Centre for Protein Structure
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Video-conferencing Centre
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Marja Mali, M. Sc.

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Aleš Cesar, B. Sc.

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Dr. Andrej Prošek
Workshops
Franc Setnikar, B. Sc.

PARTICIPATION IN THE REGIONAL DEVELOPMENT OF RESEARCH

Ljubljana Technology Park Ltd.

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

[3] until 31 January 2020 [4] since 1 February 2020

MANAGEMENT

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Director JSI
Prof. Jadran Lenarčič [1]
Prof. Boštjan Zalar [2]

Assistant to the Director
Dr. Romana Jordan [3]

Adviser
Marta Slokan, LL. B.

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Prof. Sašo Džeroski, *JSI*
Mrs. Martina Gašperlin, *Ministry for Economic Development and Technology, until 14. 9. 2020*
Prof. Primož Pelicon, *JSI*
Stojan Petrič, *Kolektor, Idrija*
Prof. Jože Pungerčar, *JSI*
Dr. Tomaž Savšek, *TPV Group, d. o. o., Novo mesto*
Mrs. Urška Zupin, *Ministry for Economic Development and Technology, since 15. 9. 2020*

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Prof. Miran Čeh
Prof. Svjetlana Fajfer
Prof. Matjaž Gams
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Prof. Nada Lavrač
Prof. Jadran Lenarčič, ***until 10. 12. 2020***
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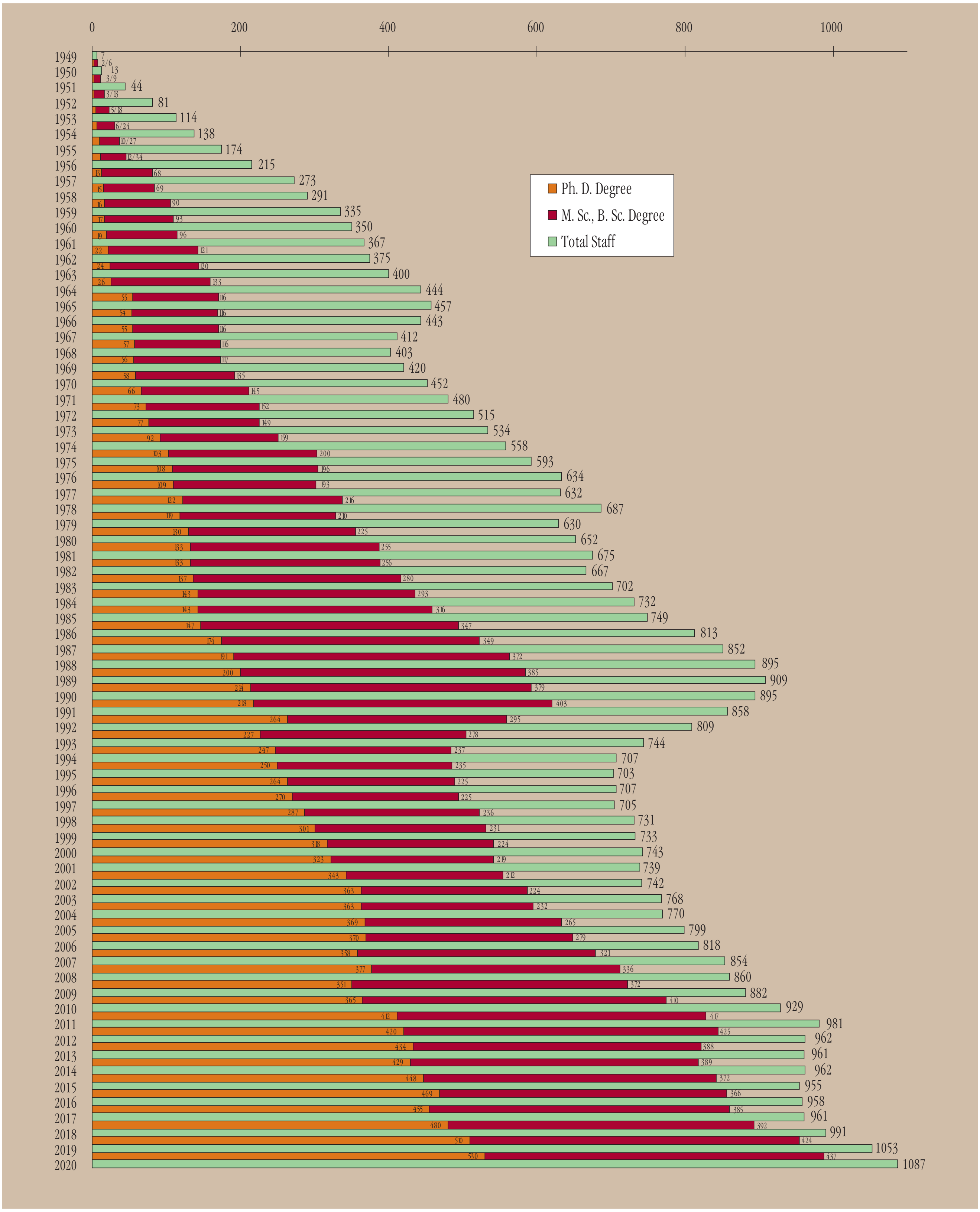
[1] until 2 July 2020, acting Director: 3 July 2020–30 November 2020
[2] since 1 December 2020
[3] until 2 July 2020, 1 September–30 November 2020 assistant to the acting Director

STAFF QUALIFICATIONS

1949-2020



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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
H2020 (EUROPEAN INSTITUTE OF INNOVATION AND TECHNOLOGY, EXCELLENT SCIENCE, EURATOM, INDUSTRIAL LEADERSHIP, SOCIETAL CHALLENGES, SPREADING EXCELLENCE AND WIDENING PARTICIPATION, SCIENCE WITH AND FOR SOCIETY)	126
ESSR (INTERREG, KC, SRIP, SPS, KPP, RZ...)	37
OTHERS (COST, IAEA, ICTP, JRC, ESA, CEF, EMPIR, ERASMUS+, LIFE+, ERA.NET, ARIMNET, ALL, PTD...)	162
TOTAL	**325**

Bilateral cooperation	No. of projects
Austria	4
Bosnia and Herzegovina	1
Germany	7
France	4
Croatia	6
Italy	3
Japan	3

Bilateral cooperation	No. of projects
Montenegro	1
Russia	1
Serbia	5
Turkey	1
USA	35
TOTAL	**71**

INTERNATIONAL COOPERATION AGREEMENT

In 2020, international cooperation agreement was signed between the Jožef Stefan Institute and Tohoku University, Sendai, Japan (F5).

COOPERATION WITH HIGHER-EDUCATION ESTABLISHMENTS

FULL-TIME FACULTY MEMBERS

Professors

1. **Prof. Denis Arčon**, University of Ljubljana, Faculty of Mathematics and Physics
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35. **Prof. Anton Ramšak**, University of Ljubljana, Faculty of Mathematics and Physics
36. **Prof. John Shawe-Taylor**, University College London, Centre for Computational Statistics and Machine Learning, London, UK
37. **Asst. Prof. Urban Simončič**, University of Ljubljana, Faculty of Mathematics and Physics
38. **Asst. Prof. Lea Spindler**, University of Maribor, Faculty of Mechanical Engineering
39. **Asst. Prof. Andrej Studen**, University of Ljubljana, Faculty of Mathematics and Physics
40. **Prof. Simon Širca**, University of Ljubljana, Faculty of Mathematics and Physics
41. **Prof. Žiga Šmit**, University of Ljubljana, Faculty of Mathematics and Physics
42. **Prof. Borut Štrukelj**, University of Ljubljana, Biotechnical Faculty and Faculty of Pharmacy
43. **Prof. Tanja Urbančič**, University of Nova Gorica
44. **Prof. Nataša Vaupotič**, University of Maribor, Faculty of Education
45. **Prof. Katarina Vogel-Mikuš**, University of Ljubljana, Biotechnical Faculty
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47. **Prof. Primož Ziherl**, University of Ljubljana, Faculty of Mathematics and Physics
48. **Asst. Prof. Dejan Žontar**, University of Ljubljana, Faculty of Health Sciences

Assistants and researchers

1. **Dr. Jure Leskovec**, Stanford University, Palo Alto, California, USA
2. **Dr. Jure Pražnikar**, University of Primorska, Faculty of Mathematics, Natural Sciences and Information Technologies, Koper
3. **Dr. Tomaž Rejec**, University of Ljubljana, Faculty of Mathematics and Physics

PART-TIME FACULTY MEMBERS

Professors

1. **Prof. Jan Babič**, University of Ljubljana, Faculty of Electrical Engineering and IPS, Ljubljana
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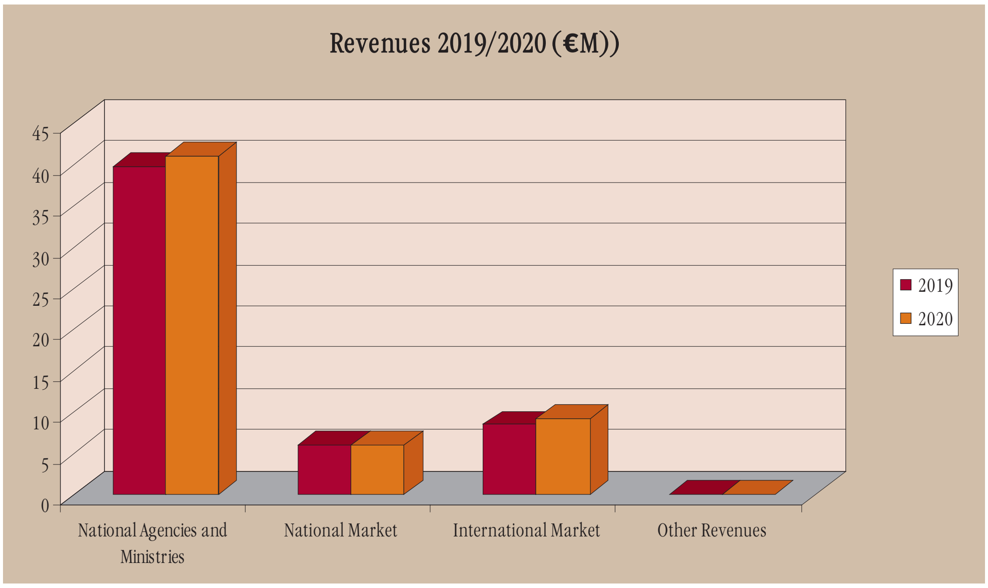
REVENUES JSI (€) AND NUMBER OF PROJECTS

	2020	Contribution 2020	2019	Contribution 2019	Index 2020/2019	No. of Projects in 2020
National Agencies and Ministries	41,157,432	72.7 %	39,744,499	73.0 %	103.6	435
National Market	6,081,337	10.7 %	6,104,020	11.2 %	99.6	363
International Market	9,235,685	16.3 %	8,501,438	15.6 %	108.6	292
Other Revenues	124,806	0.2 %	59,651	0.1 %	209.2	
TOTAL	**56,599,260**	**100.0 %**	**54,409,608**	**100.0 %**	**104.0**	**1090**



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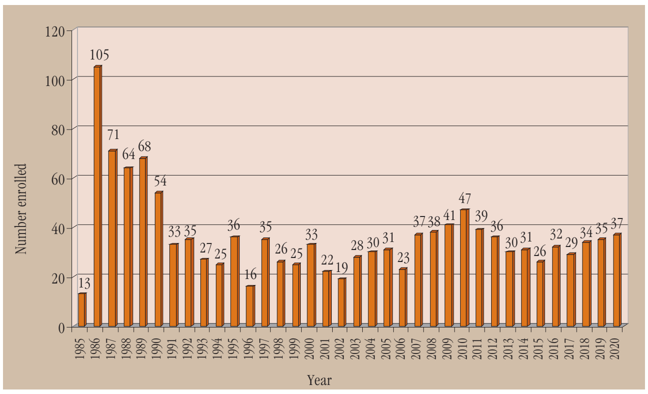

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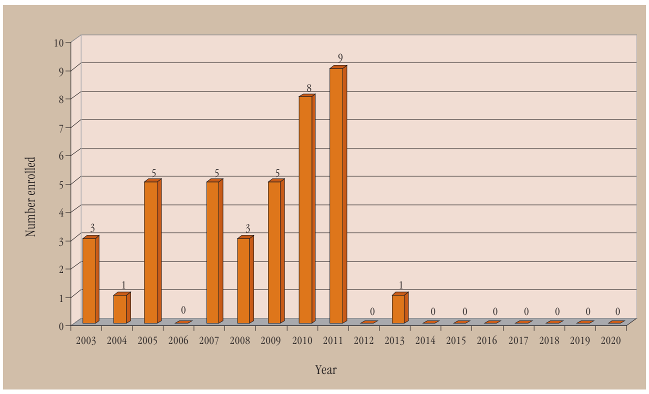

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Year	FMF		FKKT UNI LJ	FKKT UNI MB	NTF	FDV	FA	BF	FE and FRI	Other UNI LJ	FG and FERI	UNG	IPS	Total
	Physics	Mathematics												
... 1989	242	75	144					4	181	21	4			671
1990	26	5	11					2	25		1			70
1991	23	2	9					2	24	2	1			63
1992	22	3	16					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
TOTAL	490	113	452	25	13	8	4	67	504	35	22	11	87	1831

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NTF	Faculty of Natural Sciences and Engineering, University of Ljubljana
FDV	Faculty of Social Sciences, University of Ljubljana
FA	Faculty of Administration, University of Ljubljana
BF	Biotechnical Faculty, University of Ljubljana
FE	Faculty of Electrical Engineering, University of Ljubljana
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FERI	Faculty of Electrical Engineering and Computer Science, University of Maribor
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14. Gregor Papa, Barbara Koroušić-Seljak, Marko Pavlin, Device and method for acquisition and transfer of signals, GB2525403 (B), UK Patent Office, 23. 12. 2020.
15. Xinzheng Zhang, Jingjun Xu, Bin Shi, Xiaodan Xu, Yang Liu, Mengxin Ren, Wei Cai, Qiang Wu, Irena Drevenšek Olenik, Processing method and processing system for laser-induced graphene micronano structure, CN107244669 (B), State Intellectual Property Office of the P.R.C., 25. 12. 2020.
16. Gregor Primc, Miran Mozetič, Rok Zaplotnik, Alenka Vesel, Maja Ravnikar, Jana Žel, Nataša Mehle, Ion Gutiérrez-Aguirre, Arijana Filipić, David Dobnik, Procedure for inactivating virus in water, SI25811 (A), Slovenian Intellectual Property Office, 30. 09. 2020.
17. Alenka Vesel, Miran Mozetič, Rok Zaplotnik, Gregor Primc, Nina Recek, Procedure for increasing the hydrophilicity of a polymer containing fluorine, SI25862 (A), Slovenian Intellectual Property Office, 31. 12. 2020.

ART EXHIBITIONS AT THE JSI

Stojan Špegel, 13 January–5 February

Andreja Gregorič, 10 February–28 May

Bojan Golčar, 1–24 June

Miro Bone, 29 June–22 July

Mira Uršič, 27 July–2 September

Maja Šivec, 7–30 September

Bogdan Čobal, 5 October–16 December

Marjan Humar, 16 December–18 January 2021

Stojan Špegel at the opening of his exhibition

REVIEW OF PUBLICATIONS

FOR 2020

Department	Original Articles*	Books	Patent Appl. and Grants	Ph. D. Theses
Department of Theoretical Physics (F-1)	90	3		1
Department of Low and Medium Energy Physics (F-2)	76	2	1	2
Department of Thin Films and Surfaces (F-3)	13			
Department of Surface Engineering and Optoelectronics (F-4)	52	1	8	
Department of Solid State Physics (F-5)	170	6	4	4
Department of Gaseous Electronics (F-6)	37		1	
Department for Complex Matter (F-7)	55	1	2	2
Department of Reactor Physics (F-8)	75	2		3
Department of Experimental Particle Physics (F-9)	102			2
Department of Inorganic Chemistry and Technology (K-1)	18	1	1	2
Department of Physical and Organic Chemistry (K-3)	17			1
Electronic Ceramics Department (K-5)	52			2
Department for Nanostructured Materials (K-7)	71		2	2
Department for Synthesis of Materials (K-8)	25			
Department for Advanced Materials (K-9)	55			
Department of Biochemistry, Molecular and Structural Biology (B-1)	25		2	
Department of Molecular and Biomedical sciences (B-2)	15			1
Department of Biotechnology (B-3)	39			1
Department of Environmental Sciences (O-2)	94	1	2	3
Department of Automation, Biocybernetics and Robotics (E-1)	42			3
Department of Systems and Control (E-2)	28			
Artificial Intelligence Laboratory (E-3)	70	1		
Laboratory for Open Systems and Networks (E-5)	16			
Department of Communication Systems (E-6)	51	1		2
Computer Systems Department (E-7)	57		1	
Department of Knowledge Technologies (E-8)	118	1		3
Department of Intelligent Systems (E-9)	63	2	2	1
Department of Reactor Engineering (R-4)	46	1	1	
Reactor Infrastructure Centre (RIC)	14			1
Energy Efficiency Centre (EEC)	9	1	1	1
Centre for Electron Microscopy and Microanalysis (CEMM)	3			
Milan Čopič Nuclear Training Centre (ICJT)	6			1
Radiation Protection Unit (SVPIS)	1			
Centre for Technology Transfer and Innovation (CTT)	11	1		
Jožef Stefan Institute	1418	20	23	39

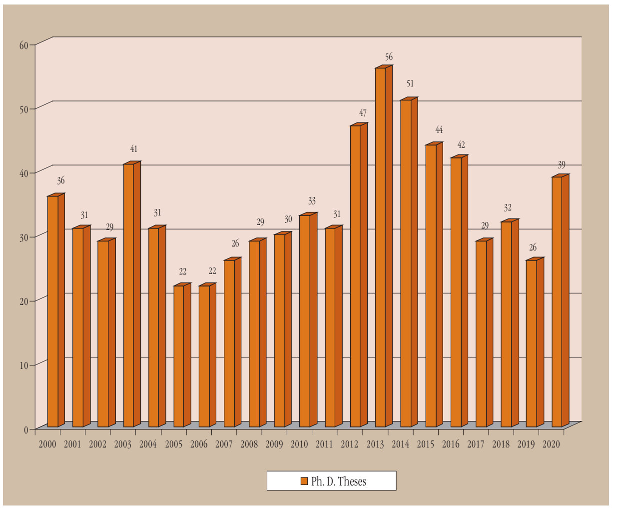
* Articles in Journals and Conference Proceedings, and Chapters in Books

COMPLETED THESES

UNTIL 2020

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
TOTAL	1251



AWARDS AND APPOINTMENTS

AWARDS MADE TO JSI RESEARCHERS BY THE REPUBLIC OF SLOVENIA

Zois and Puh Awards and Zois Certificate of Recognition

Barbara Malič
Presented with the Zois Award for outstanding scientific achievements in the field of electrocaloric ceramics

Andrej Filipčič and Marko Zavrtanik
Presented with the Zois Award for outstanding scientific achievements in research of extreme energy cosmic particles

Samo Kralj
Presented with the Zois Certificate of Recognition for outstanding research achievements in the field of soft-matter physics

Janko Petrovčič
Presented with the Puh Award for outstanding achievements in the field of innovative electronic systems

JSI AWARDS AND APPOINTMENTS

Blinc Award

Danilo Zavrtanik
Blinc Award for lifetime achievement in physics

Giovanni De Ninno
Blinc Award for the contribution in Nature Photonics: Photoelectric effect with a twist

Jernej Fesel Kamenik
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 :

Matjaž Gomilšek
Quantum spin liquids on geometrically frustrated kagome lattices

Gregor Posnjak
Topological formations in chiral nematic droplets

Janja Vidmar
Quantification and sizing of metal-based nanoparticles in the environmental and biological samples

JSI Director's fund

Igor Vaskivskyi
for the project entitled for the Laboratory for 4D Resonance Magnetic Spectroscopy

OTHER SELECTED AWARDS TO JSI RESEARCHERS

Centre for Knowledge Transfer in Information Technologies (CT3), as part of the international mentoring programme for open education called "Open Education for a better world - OE4BW", completed the third cycle with 82 projects developed and received the Award for Excellence for efforts from the Open Education Global Community.

Julio Benavides, **Oriol Costa Garrido**, **Gonzalo Jimenez**, **Leon Cizelj**, Best poster award (NENE2020 conference, Portorož) Nuclear Society of Slovenia, Thermo-mechanical Analysis of a Dry Storage System

Andreja Benčan Golob, **Andraž Bradeško**, **Mirela Dragomir**, **Goran Dražić**, **Maja Makarovič**, **Barbara Malič**, **Uroš Prah**, **Tadej Rojac**, **Hana Uršič Nemevšek**, Achievement Excellent in Science 2020 for Innovative approaches to the control of functional responses of multiferroics, Slovenian Research Agency

Jernej Birk, **Domen Hočevar**, **Kaja Rangus**, Krka Award for undergraduate research assignments, Krka, d.d., Use of microthermophoresis to determine sugar binding to rCnSL-B2 isolectin (mentors, Janja Pust, Jerica Sabotič, Ana Mitrović)

Klara Čebular, Krka Award 2020 for her PhD thesis entitled "Transformations of oxygen functional groups in organic molecules mediated by molecular iodine or/and N-halo compounds".

Urša Čerček, Faculty of Pharmacy student Prešeren award 2020, Ljubljana, Faculty of Pharmacy, Effect of cold atmospheric pressure plasma on formation of stress granules in the selected stable cell line.

Urša Čerček, Krka recognition for undergraduate and postgraduate research work, Krka, Krka, Effect of cold atmospheric pressure plasma on formation of stress granules in the selected stable cell line**.**

Matjaž Dlouhy, First prize in the category best posters and lectures for the poster entitled "Adsorption of imidazole on Cu (111), covered with corrosion-important species" at the 26th annual meeting of the Slovenian Chemical Society entitled "Slovenian Chemical Days 2020", September 16–18, 2020.

Mirela Dragomir, Seal of Excellence for project application QMAT – Towards Quantum States of Matter via Chemistry under Ambient and Extreme Conditions, European Commission

Sabina Drofenik, Prešeren Prize for Students of the University of Ljubljana 2020, University of Ljubljana, award-wining bachelor thesis entitled 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 Igor Križaj)

Tome Eftimov, **Rok Hribar**, **Peter Korošec**, **Gašper Petelin**, **Gorjan Popovski**, **Urban Škvorc**, took 1st place in the competition organized as part of the GECCO 2020 (GECCO Open Optimization Competition 2020), "Deep statistic: more robust performance statistics for single – objective optimization benchmarking". The award was given by The Nevergrad and the IOHprofiler team (https://github.com/facebookresearch/nevergrad/blob/master/docs/opencompetition2020.md

B. Evkoski, **I. Mozetič**, **N. Ljubešić**, **P. Kralj Novak**, Best lightning presentation award: Evolution of political polarization on Slovenian Twitter, Complex Networks and their Applications, Madrid, Spain, December 1-3, 2020.

Martin Gjoreski, **Vladimir Kuzmanovski and Marko Bohanec**, best paper award for the paper "Generating alternatives for DEX models using Bayesian optimization", Slovenian Conference on Artificial Intelligence, SCAI 2020, Ljubljana, 6–7 October 2020.

Primož Godec, **Matjaž Pančur**, **Nejc Ilenič**, **Andrej Čopar**, **Martin Stražar**, **Aleš Erjavec**, **Ajda Pretnar**, **Janez Demšar**, **Anže Starič**, **Marko Toplak**, **Lan Žagar**, **Jan Hartman**, **Hamilton Wang**, **Riccardo Bellazzi**, **Uroš Petrovič**, **Silvia Garagna**, **Maurizio Zuccotti**, **Dongsu Park**, **Gad Shaulsky**, **Blaž Zupan**, Best Research Achievements of the University of Ljubljana 2020, University of Ljubljana, for publication: Democratized image analytics by visual programming through integration of deep models and small-scale machine learning, Nature Communications 10 (2020): 4551.

Heli Jantunen, Yushan Scholar Award, Yushan, Taiwan, Ministry of Education (MOE), ROC Taiwan, Ultra-low temperature co-firing ceramics.

Eva Jarc Jovičić, 50th Krka Prizes, Krka recognition with special honours for the research work, Krka d.d., for the doctoral thesis entitled The role of lipid droplets in cancer cell stress resistance

Ita Junkar, **Metka Benčina**, **Janez Kovač**, **Miran Mozetič**, **Rok Zaplotnik**, Innovation of the Year, virtual, Regional Virtual Fair on Innovation and Entrepreneurship "Sarajevo 2020", "Method for treatment medical devices made from nickel-titanium (NiTi) alloys".

The winner of Zois Award Prof. Barbara Malič. Photo: Nebojša Tejić/STA

The winners of Zois Awards Prof. Andrej Filipčič, Prof. Samo Stanič and Prof. Marko Zavrtanik. Photo: Nebojša Tejić/STA

Ita Junkar, Excellent in Science 2020 Achievement (Odlični v znanosti 2020), Ljubljana, Scientific Council of Slovenian Research Agency (ARRS), "Method of treatment of tools used for isolation of microvesicles, nanovesicles and exosomes".

Stefan Kalabakov, Simon Stankoski, Nina Reščič, Andrejaana Andova, Ivana Kiprijanovska, Vito Janko, Martin Gjoreski, Mitja Luštrek, SHL Challange – Sussex-Huawei Locomotion and Transportation Recognition Challenge, 3rd Place Award, virtual, Hristijan Gjoreski, University of Sussex (UK) & Ss. Cyril and Methodius University (MK), Lin Wang, University of Sussex (UK), Daniel Roggen, University of Sussex (UK), Kazuya Murao, Ritsumeikan University (JP), Tsuyoshi Okita, Kyushu Institute of Technology (JP), Mathias Ciliberto, University of Sussex (UK), Paula Lago, Kyushu Institute of Technology (JP), method for recognition of locomotion activity from smartphone sensors

The winner of Puh Award Dr. Janko Petrovčič. Photo: Nebojša Tejić/STA

Jan Kejžar, Krka's recognition for the master's thesis: Comparison of dietary supplements from algae: antioxidant potential and isotopic composition

Boshko Koloski, Senja Pollak and Blaž Škrlj, participation in the computer competition in the field of profiling of authors of PAN texts, where they achieved 2nd place in the field of profiling of celebrities (out of 66 groups) and 3rd place in the field of multilingual classification of users who share fake news

Bor Kos, Best Poster Award, Portorož, Slovenia, "29th International Conference Nuclear Energy for New Europe - NENE 2020", September 2020, for a poster "TCV Tokamak Neutron Shielding Assessment and Upgrade"

Domen Kotnik, Faculty Prešeren Award for MSc Thesis, Ljubljana, University of Ljubljana, Faculty of Mathematics and Physics, January 2020

Jan Kren, Dean's Award for Outstanding Academic Achievement UL FMF, University of Ljubljana

Tadej Krivec, awarded with the PCT technology network award (Process Control Technology) for his master's thesis entitled "Complex event processing in production process monitoring", Ljubljana

Rok Krpan, Best Video Presentation–European Award (International conference ICONE 2020, virtual) American Society of Mechanical Engineers, Simulations of Experiments on Isothermal Containment Atmosphere Mixing Caused by Vertical Injection

Neja Kuret, Krka Award, Krka, d.d., Effect of kokaprin lectin on pathogenic and probiotic bacteria (Mentors: Anja Klančnik, Jerica Sabotič)

Aleš Lapanje, Slovenian Research Agency - Excellent in Science 2020: The most visible research achievements inspiring young generations. Area: Biotechnology. Title: How we made a live protective coating.

Zorica Latinović, 50th Krka Prizes, Krka recognition with special honours for the research work, Krka d.d., for the Doctoral Thesis entitled Components of the nose-horned viper venom that affect cardiovascular system

Adrijana Leonardi, Kity Požek, Igor Križaj, 7th International Toxinology Meeting, Poster Award for the poster entitled Biochemical and functional characterization of the first member of the new P-IIIe subclass of snake venom metalloproteinases

Mirjana Malnar, Award for presentation of research achievements in terms of scientific quality and their applicability, 12th Jožef Stefan International Postgraduate School Students' Conference and 14th CMBE day, presentation of research work

Luka Medic, Prešeren Award, University of v Ljubljana, master's thesis "Topological quantization of the transconductance in a Josephson junction with the Rashba interaction"

Alenka Mertelj, Mid Career Research Excellence Award, ILCS (The International Liquid Crystal Society) for discovery of both magnetic and electric polar order in nematic phase and new spatially modulated splay nematic phase that has macroscopic electric polarization, 2020

Simon Mezgec won 2nd place in the Food Recognition Challenge competition organized by AIcrowd (https://www.aicrowd.com/challenges/food-recognition-challenge/leaderboards?challenge_round_id=261

Dragan Mihailović, Damjan Svetin, Anže Mraz, Rok Venturini, Gold medal at the 18th International Innovation Exhibition ARCA 2020 for poster Innovative superconductor-based memory device and method for its operation, using a switchable resistive element suitable for superconducting computing – compatible with superconducting flex-quantum electronics, Zagreb, Croatia

Dragan Mihailović, Damjan Svetin, Anže Mraz, Rok Venturini, Silver medal at the 1st virtual fair of innovation and entrepreneurship "Sarajevo 2020" for Memory device and method for its operation, Startup studio Fondacije Mozaik in Sarajevo Business Forum (SBF), Bosna in Hercegovina, 24. 11. 2020

Clément Picard, Vito Janko, Nina Reščič, Martin Gjoreski, Mitja Luštrek, The Cooking Activity Recognition Challenge 1st Place Award, virtual / Kitakyushu, Japan, ABC Conference, method for recognition of cooking activities with sensors

Tim Podlogar, Gatorade Sports Science Institute Award, Köln, Germany, 25. ECSS Congress European College of Sport Science (virtual), Effectiveness of combined galactose-glucose ingestion as compared to galactose or glucose only on post-exercise muscle glycogen repletion

Gregor Primc, Miran Mozetič, Rok Zaplotnik (Jožef Stefan Institute), in collaboration with David Dobnik, Matevž Dular, Arijana Filipić, Ion Gutierrez-Aguirre and Martin Petkovšek, Prize for the Best Innovation with Commercial Potential in 2020, Ljubljana, 13th International Technology Transfer Conference for the innovation, "A scalable method for eco-benign destruction of waterborne microorganisms".

Emanuela Senjor, 3rd place UCLA Research Day 2020 Poster Competition, Los Angeles, USA, University of California Los Angeles, School of Dentistry

Maj Smerkol, Best paper award at People and Environment, 23rd International Multiconference Information Society, IS 2020, Ljubljana, Jozef Stefan Institute, Traffic Simulation Software in the Context of Mobility Policy Support System

Matjaž Spreitzer, Srečo Škapin, Silver award of the CCIS for the innovation TCG Autoskimm, Maribor, Chamber of Commerce and Industry of Slovenia, Development of automatic slag skimming process to reduce aluminum losses and ensure reproducible melt quality.

Matjaž Spreitzer, Srečo Škapin, Silver award of the CCIS for the innovation New super-light and super hard engineering materials, Maribor, Chamber of Commerce and Industry of Slovenia, Development of a laboratory-verified synthetic pathway for the production of lightweight, super-solid advanced materials based on Al-Mg-B-Ti.


The Blinc award is conferred by the Jožef Stefan Institute and the Faculty of Mathematics and Physics, University of Ljubljana.

The above photomontage shows winners of the Blinc awards: Prof. Danilo Zavrtanik (top left), Prof. Giovanni De Ninno (top centre) and Prof. Jernej Fesel Kamenik (top right). Prof. Nataša Vaupotič, President of Blinc Award Commission (left centre), Prof. Jadran Lenarčič, Director of the JSI (centre), Prof. Anton Ramšak, Dean of the Faculty of Mathematics and Physics (right centre) and Prof. Robert Repnik, Director of the Slovenian Research Agency ARRS (bottom left).

Pia Starič, **Ita Junkar**, **Miran Mozetič**, **Katarina Vogel-Mikuš**, Best Paper Award, virtual, Sciforum, The 1st International Conference on "Green" Polymer Materials 2020, "Bio-Polymers in the World of Plasma: Effects of Cold Plasma on Seed Surface".

Danilo Suvorov, **Srečo Škapin**, **Marija Vukomanović**, Special prize for innovations for economy, Ljubljana, Center for technology transfer and innovation JSI, Contact-based, leaching-free antimicrobial textile Silver-free, wearable germ protection.

Nina Šiškovič, Biotechnical Faculty's Prešeren Award for 2020, Determination of volatile organic compounds in truffles

Sašo Šturm was in August 2020 elected as a member in Executive Board of European Microscopy Society (EMS). The EMS is an umbrella organization that brings together all national microscopy societies. Sašo Šturm was proposed by the Slovene Society for Microscopy (SDM) Executive Board and thus the Slovenian representative in the EMS Executive Board was elected for the first time.

Jan Šuntajs, Prešeren Award, University of v Ljubljana, master's thesis "Spectral properties of the t-J model and many-body localization"

Žiga Tkalec, Best Poster Award on Exposome Symposium, New York, USA, Mount Sinai Institute for Exposomic Research, Development of an analytical method for nontargeted screening for organic contaminants in human urine.

Špela Trafela was awarded by L'Oréal-UNESCO National Programme for Women in Science in 2020 in recognition of her fundamental and applied research. She has developed nanostructured sensor platforms-based on $Ni(OH)_2$/NiOOH-Ni redox system for electrochemical detection of formaldehyde in alkaline media.

Tea Tušar, Best Paper award at Human-Computer Interaction in Information Society, 23rd International Multiconference Information Society, IS 2020, Ljubljana, Jožef Stefan Institute, Interactive visualization of the Slovenian budget with the Sankey diagram

Lara Ulčakar, L'Oreal Adria and Slovene committee at UNESCO award

Alenka Vesel received the WIPO medal for inventors awarded by the Slovenian Intellectual Property Office in collaboration with the World Intellectual Property Organization for her innovations and innovative activities.

Damir Vrančić, the silver award for innovation went to Danfoss Trata d.o.o. for Virtus iSET/iNET innovation of smart-operated pressure regulators and valves for district heating. A member of the awarded group was our Department member. Chamber of Commerce and Industry of the central Slovenia region for the best innovations for the year 2020, Ljubljana

Andrej Žohar, Young Author Award for the best contribution, Portorož, Slovenia, "29th International Conference Nuclear Energy for New Europe - NENE 2020", September 2020, for an article "Water Activation Experiment and Calculations at JSI TRIGA Research Reactor"

Editorial Board from a prominent journal Green Chemistry, has selected a paper by **Xuan Xu**, **Sašo Šturm**, **Zoran Samardžija**, **Janez Ščančar**, **Katarina Marković**, **Kristina Žužek Rožman**, all from the Jožef Stefan Institute entitled "A facile method for the simultaneous recovery of the rare-earth elements and transition metals from Nd-Fe-B magnets" as a 2020 HOT Green Chemistry article. The paper is a result of the ITN-MSCA project DEMETER, Training Network for the Design and Recycling of Rare–Earth Permanent Magnet Motors and Generators and Full Hybrid and Electric Vehicles [2015-2019], for which funding is gratefully acknowledged.

KNOWLEDGE TRANSFER

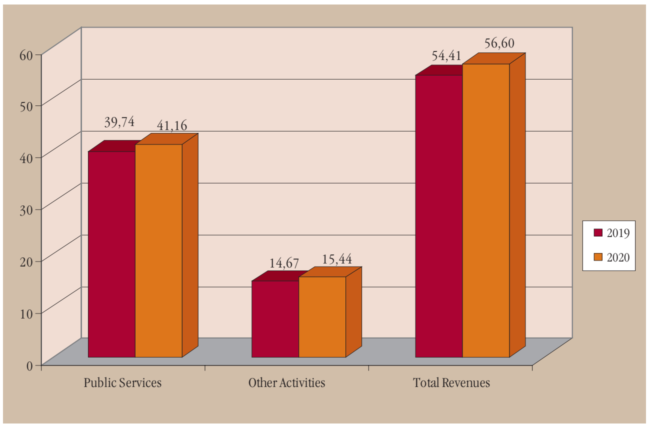
The JSI pays a lot of attention to furthering its links with industry. In keeping with European aims and the objectives of the Slovenian government, the JSI organized several important meetings on the subject of cooperation with enterprises and industry. In this way the JSI introduced a new method of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

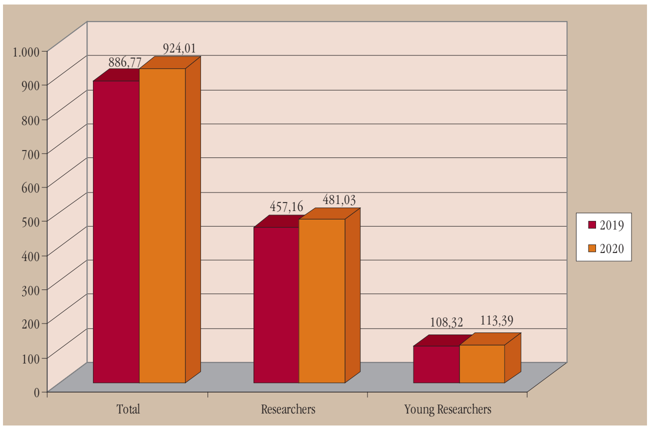
1. Agency for Radwaste Management, Ljubljana
2. Arctur, d.o.o., Nova Gorica
3. Arhel projektiranje in inženiring, d.o.o., Ljubljana
4. Bias Variance Labs, d.o.o., Ljubljana
5. Biodelta, d.o.o., Ljubljana
6. Central Technical Library at the University of Ljubljana, Ljubljana
7. Cosylab, d.d., Ljubljana
8. Elan, d.o.o., Begunje na Gorenjskem
9. Elektro Celje, d.d., Celje
10. Elektro Energija, d.o.o., Ljubljana
11. Elektro Ljubljana, d.d., Ljubljana
12. Elvez, d.o.o., Višnja Gora
13. Ema, d.o.o., Celje
14. Eurofins ERICo Slovenija, d.o.o., Velenje
15. Event Registry, d.o.o., Ljubljana
16. FerroČrtalič, d.o.o., Dolenjske Toplice
17. Gabrijel Aluminium, d.o.o., Grosuplje
18. Gemis, d.o.o., Brežice
19. Gen energija, d.o.o., Krško
20. Grid Instruments, d.o.o., Ljubljana
21. Helios, d.o.o., Domžale
22. Induktio, d.o.o., Ljubljana
23. Infinite, d.o.o., Limbuš
24. InoVine, d.o.o., Ljubljana
25. Irgo Consulting, d.o.o., Ljubljana
26. Jems, energetska družba, d.o.o., Ljubljana
27. Keko - Oprema, d.o.o. Žužemberk
28. KMZ - Zalar Miran s.p., Ljubljana
29. Kolektor Group, d.o.o., Idrija
30. Krško Nuclear Power Plant, Krško
31. Lama avtomatizacija, d.o.o., Dekani
32. Lek, d.d., Ljubljana
33. Luka Koper, d.d., Koper
34. Matima, d.o.o., Postojna
35. Melamin kemična tovarna, d.d., Kočevje
36. Ministry of Agriculture, Forestry and Food, Ljubljana
37. Ministry of Defence, Ljubljana
38. Ministry of Finance, Ljubljana
39. Ministry of Health, Ljubljana
40. Ministry of the Environment and Spatial Planning, Ljubljana
41. Nanos Scientificae, d.o.o., Ljubljana
42. Nanotul, d.o.o., Ljubljana
43. National Education Institute, Ljubljana
44. National Institute of Biology, Ljubljana
45. National Institute of Chemistry, Ljubljana
46. Or-el, d.o.o., Kobarid
47. Paradajz, d.o.o., Turnišče
48. Plinovodi, d.o.o., Ljubljana
49. Quintelligence, d.o.o., Ljubljana
50. Razvojni center eNeM Novi Materiali, d.o.o., Zagorje ob Savi
51. Republic of Slovenia Statistical Office, Ljubljana
52. RLS Merilna tehnika, d.o.o., Komenda
53. SID banka, d.d., Ljubljana
54. Slovenian Beekeeper's Association, Lukovica
55. Slovenian National Building and Civil Engineering Institute, Ljubljana
56. Slovenian Reserch Agency, Ljubljana
57. Slovensko društvo ljubiteljev kemije, Ljubljana
58. Sonce energetika, d.o.o., Ljubljana
59. SRC, d.o.o., Ljubljana
60. STA, d.o.o., Ljubljana
61. Steklarna Hrastnik - Opal, d.o.o., Hrastnik
62. Stelem, d.o.o., Žužemberk
63. Tanin Sevnica, d.d., Sevnica
64. TH Re-Mining, d.d., Ljubljana
65. University Medical Center Ljubljana, Ljubljana
66. University Medical Center, Ljubljana
67. University of Ljubljana, Ljubljana
68. University of Maribor, Maribor
69. Weiler Abrasives, d.o.o., Maribor

INSTITUTE IN NUMBERS 2019–2020

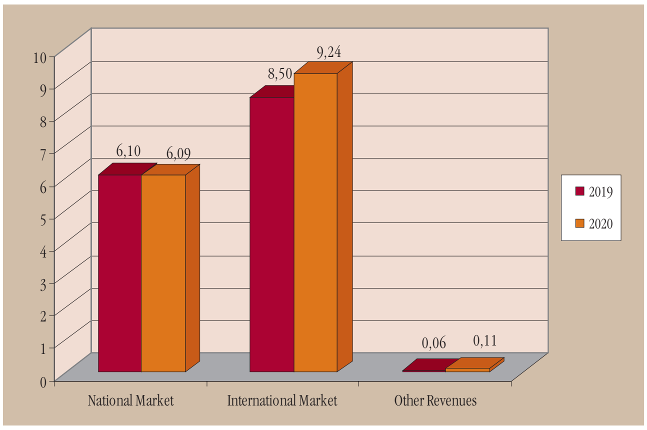
COMPARISON OF REVENUES (€M)



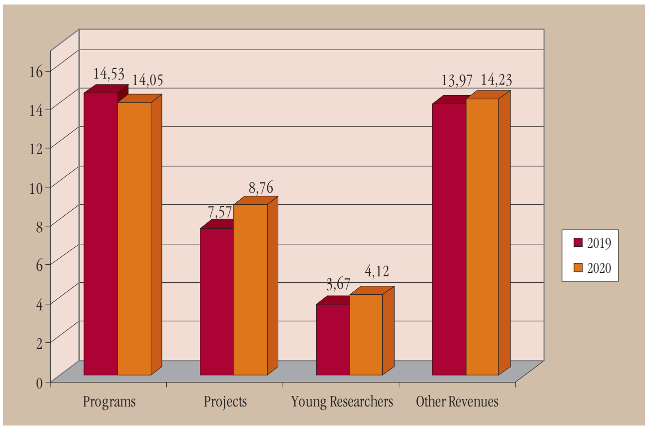
EMPLOYEES (FTE)



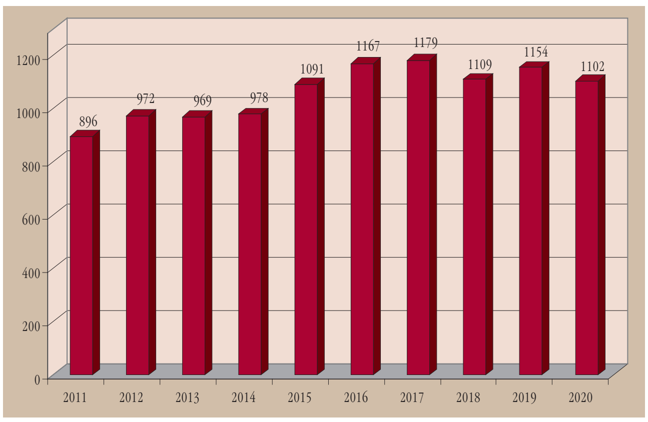
REVENUES FROM OTHER ACTIVITIES (€M)



REVENUES FROM PUBLIC SERVICES (€M)

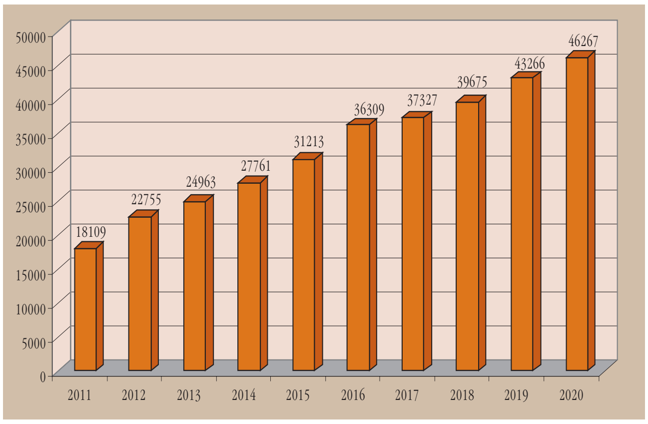


NUMBER OF PUBLICATIONS IN THE WEB OF SCIENCE*



* retrieved 9 August 2021

NUMBER OF CITATIONS IN THE WEB OF SCIENCE*

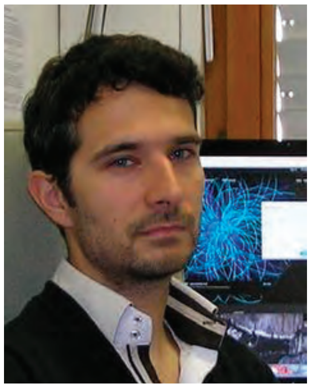


* retrieved 9 August 2021

RESEARCH DEPARTMENTS

DEPARTMENT OF THEORETICAL PHYSICS F-1

In 2020 members of the programme group THEORY OF NUCLEUS, ELEMENTARY PARTICLES AND FIELDS continued with research in the area of hadronic physics, quantum chromodynamics, effective field theory of electroweak decays of mrsons, unified theory and precise calculation in three-body systems.



Head:
Prof. Jernej Fesel Kamenik

We described a technique of Latent Dirichlet Allocation to learn the underlying structure of high-energy particle collider events directly from the data, without having a particular theoretical model in mind. We used it to extract the latent probability distributions describing the learned underlying structure of collider events using two example scenarios to learn the latent structure of di-jet event samples made up of QCD background events and either top-pair production or hypothetical $W' \rightarrow (\varphi \rightarrow W W)W$ signal events.

We investigated the consequences of deviations from the Standard Model observed in $b \rightarrow s\mu\mu$ transitions for flavour-changing neutral-current processes involving down-type quarks and neutrinos. We derived the relevant Wilson coefficients within an effective-field-theory approach respecting the SM gauge symmetry, including right-handed currents, a flavour structure based on approximate U(2) symmetry, and assuming only SM-like light neutrinos, and discussed resulting correlations among $B \rightarrow K(*)\nu\nu$ and $K \rightarrow \pi\nu\nu$ branching ratios.

We considered different aspects of New Physics. We studied leptoquarks, singlets S1 and U1, relying on the low-energy flavour physics measurements, LHC, and the IceCube neutrino data. We analysed the chiral enhancement required to explain the muon (electron) anomalous magnetic moment, using models of leptoquarks.

For the CP-odd pseudoscalar coupling between the Higgs boson and the top quark we have employed machine-learning optimization methods to improve the sensitivity at the LHC and future colliders. In models addressing the lepton universality violation in the measurement of $R_K^{(*)}$ we presented a method to test for the presence of CP-odd couplings of new physics close to the narrow charmonium resonance in the decay $B \longrightarrow K\ J/\psi \longrightarrow K\mu^-\mu^+$. In models with scalar leptoquarks that explain violation of lepton universality we considered the possibility to embed them in a dark-matter model with a heavy scalar singlet that can annihilate into pairs of leptoquarks.

We performed a detailed study of the production of type-II seesaw scalars production at hadron colliders. To this end, we developed a model implementation, which includes mixings, all the scalar couplings and chromodynamic one-loop counterterms. This allowed us to calculate the cross-sections beyond the leading order. We launched the Find Bounce tool in the Mathematica environment, which allows for a fast, efficient, reliable and arbitrary precise evaluation of the lifetime of metastable states in quantum and thermal field theories. We found an exact solution for the false vacuum decay at one loop in a bi-quartic potential.

Asymptotically safe quantum field theories have a non-trivial UV fixed point. We proposed a holographic picture of a simple asymptotically safe quantum field theory in non-integer spacetime dimensions by assuming that the UV and infrared (IR) conformal dynamics can be described by AdS spaces. The approach is similar in spirit to the one employed for holographic QCD.

We performed one of the first ab-initio theoretical studies of the exotic hadrons *Zb* composed of four valence quarks *bb-bar du-bar*. Two interesting hadrons of this kind were experimentally discovered in 2011 by the Belle collaboration. The heavy quarks were treated as static of our lattice QCD simulation, since this system is too challenging for a completely rigorous treatment.

- **We described a technique of Latent Dirichlet Allocation to learn the underlying structure of high-energy particle collider events directly from the data.**
- **We have explained $(g-2)\mu,e$ using leptoquarks and considered the impact of new physics in the $b \rightarrow s\mu\mu$ transitions on $B \rightarrow K(*)\nu\nu$ and $K \rightarrow \varpi\nu\nu$.**
- **In models addressing the anomaly in measurements of lepton universality $R_K^{(*)}$, we have proposed a measurement close to the charmonium resonance in the decay $B \longrightarrow K\ J/\psi \longrightarrow K\mu^-\mu^+$ that would reveal CP-odd components of new physics.**
- **We launched FindBounce, a Mathematica tool that allows for a fast, efficient, reliable and arbitrary precise evaluation of the lifetime of metastable states in quantum and thermal field theories with arbitrary multi-field potentials.**
- **We proposed to describe the gauge sector of an asymptotically safe field theory in d = 4–epsilon dimensions as a scalar theory on fixed AdS in (d + 1)-dimensions using the holographic dictionary.**
- **We established that the existence of the exotic tetraquarks *Zb = b-bar bdu-bar* is related to the significant attraction between mesons *B* and *B*-bar* at small distances.**
- **We have demonstrated the subset of coefficients of analytical approximations of the local behaviour of Coulomb three-body wave functions and their integrals that can be obtained analytically, and the remainder that requires a three-body method incorporating correct limits.**

Our results indicate that the existence of the exotic hadrons *Zb* is related to the significant attraction between mesons *B* in *B**-bar at small distances.

In the Coulomb three-body problem we studied analytical approximations for the radial or hyperradial dependence of one-electron and total density integrals for two-electron systems with nuclear charges Z = 1- 5. Using our own numerical method, CFHHM (Correlation FunctionHyperspherical Harmonic Method), we calculated the coefficients of analytical approximations not obtainable analytically. We calculated the critical points of the expectation values of delta functions and analytical approximations of the three-body wave function in collinear configurations. We demonstrated the significance of the fact that CFHHM includes analytical structure of the Fock expansion guaranteeing correct limits at small separations.

Some outstanding publications in the past year

1. Dillon, Patrick B., Faroughy, Darius Alexander, Kamenik, Jernej, Szewc, M. Learning the latent structure of collider events. *The journal of high energy physics*, ISSN 1029-8479, 2020, vol. 2020, no. 10, str. 206-1-206-47, doi: 10.1007/JHEP10(2020)206. [COBISS.SI-ID 36636419]
2. Doršner, Ilja, Fajfer, Svjetlana, Sumensari, Olcyr. Muon g - 2 and scalar leptoquark mixing. *The journal of high energy physics*, ISSN 1029-8479, Jun. 2020, vol. 2020, art. no. 89, 18 str., ilustr., doi: 10.1007/JHEP06(2020)089. [COBISS.SI-ID 20330243]
3. Prelovšek, Saša, Bahtiyar, Hüseyin, Petković, Jan. Zb tetraquark channel from lattice QCD and Born-Oppenheimer approximation. *Physics letters. Section B*, ISSN 0370-2693. [Print ed.], Jun. 2020, vol. 805, art. no. 135467, 5 str., ilustr., doi: 10.1016/j.physletb.2020.135467. [COBISS.SI-ID 14970883]

Awards and appointments

1. Prof. Dr. Jernej Fesel Kamenik, Robert Blinc award for physicists at the start of their career, Faculty of Mathematics and Physics, University of Ljubljana

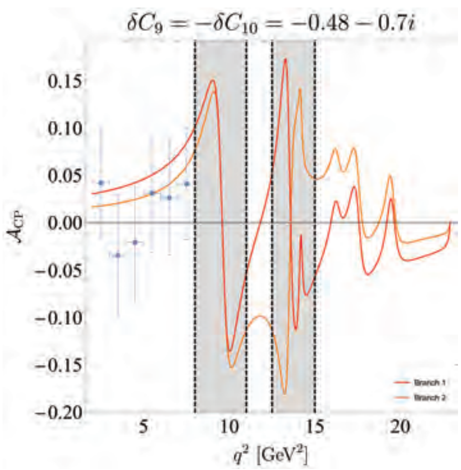


Figure 1: Prediction of direct CP asymmetry (red and orange lines) for two possible strong phases, compared with measured points by LHCb. We propose measurements in the region below the resonance, where the asymmetry attains its maximum value.

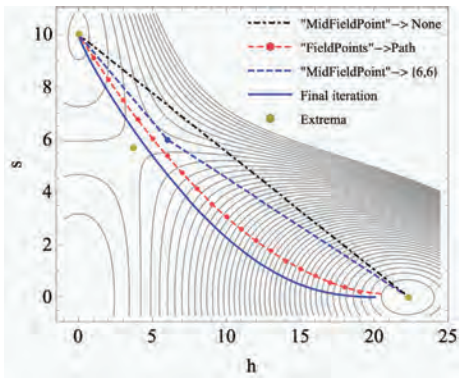


Figure 2: Calculation of the false vacuum decay rate in a two-field potential, where the solid blue line shows the final path. The black line is the straight line ansatz connecting the two minima and a middle point set by hand, red is a parabola, and blue dashed is the connected saddle point.

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

Within the framework of the theory of superconductivity we have investigated a disordered chain hosting quantum particles which form bipolarons due to coupling to magnetic excitations. We have shown that disorder can increase or decrease the binding energy, depending on the kinetic energy of the particles as well as on the density of bipolarons and the range of pairing interactions. We have computed the static and dynamic properties of an electron coupled to hard-core-boson degrees of freedom. The polaron, an electron dressed with hard-core-boson excitations, remains light even in the strong-coupling limit as its effective mass remains of the order of the free-electron mass. While the investigated model bears a resemblance to the Holstein model, we point out many important differences that originate from the binary hard-core-boson excitation spectrum, which in turn mimics spin-1/2 degrees of freedom.

- **In cooperation with experimentalists, we showed that the Heisenberg spin model on kagome lattice captures well the measured thermodynamic properties of the novel spin-liquid material YCuOHCl.**
- **We have investigated high-temperature spin transport in the Hubbard model and found a temperature-non-monotonic spin-diffusion constant.**
- **By studying the robustness of quantum chaos in disordered spin chains we introduced a new method to detect the ergodicity breaking transition in many-body quantum systems.**
- **Semiconductor-superconductor hybrid nanowires with embedded quantum dots have Coulombic sub-gap states.**
- **We calculated the resistivity of the iron in the inner Earth's core, taking both the lattice deformation due to vibrations and the electron-electron correlation effects into account.**
- **We studied the Kibble-Zurek behaviour in disordered Chern insulators.**
- **Numerical simulations of microscopic interactions in bio-social stochastic processes of spreading SARS-CoV-2 viruses reveal the background of successful social locking.**

We continued the investigations of frustrated spin models, which do not reveal any order and are characterized as spin liquids. We introduced an effective reduced model, which reproduces the properties of the Heisenberg model both on triangular and kagome lattices. We evaluated numerically the thermodynamic quantities, such as the entropy and magnetic susceptibility, for several planar frustrated spin models. We showed that the corresponding (Wilson) ratio behaves universally in the regime of spin liquids, vanishing at low temperatures. In cooperation with experimentalists, we showed that model results capture well the measured properties of novel spin-liquid material YCuOHCl

Within the framework of correlated electron systems we studied quantum models related to the phenomenon of many-body localization and anomalous relaxation. We showed that particle on a disordered ladder, coupled to hard-core bosons, exhibits sub-diffusive transport at large enough disorder, while in the limit of planar system the relaxation remains always diffusive. Furthermore, we have analysed in detail the correlations in the Hubbard model, including autocorrelations of charge, spin and energy or heat currents. Using the Nernst-Einstein relation we have shown that the spin diffusion obtains a non-monotonic temperature dependence. We further showed a discrepancy between the theory and the experiment on cold atoms.

Within the theory of dynamics of many-body quantum systems we have studied the impact of conserved quantities on the eigenstate thermalization hypothesis. We introduced a method to construct observables, which are not "similar" to conserved quantities. We also studied the robustness of quantum chaos in disordered spin chains. We introduced a new method to detect the ergodicity breaking transition in many-body quantum systems. We have introduced the cost-function-minimization approach to finding the scaling solutions for various spectral observables. We introduced the spectral form factor that can serves as a new probe for the detection of the transition between an ergodic and many-body localized phase.

The excitonic insulator is a quantum state of matter characterized by the spontaneous Bose-Einstein condensation of excitonic in a macroscopic coherent state. We show how nonlinear optical response, namely, second harmonics, can be used for the spectroscopy of collective response including the amplitude (Higgs) and the phase (Goldstone) mode. We propose concrete optical experiments based on solid-state physics to simulate the Higgs and the Goldstone dynamics.

We studied the physics of a semiconducting nanowire with an epitaxial superconducting layer coupled to an interacting quantum dot. We developed a new numerical technique for solving the corresponding theoretical model, i.e., a quantum impurity problem with an interacting superconducting bath with explicit pairing and charge-repulsion terms. We systematically explored the physics of this problem. In collaboration with an experimental group at QDev at the University of Copenhagen, we applied this approach to model an actual device, finding an excellent regime in the most interesting (and most demanding) regime of intermediate coupling. We also studied other realisations of magnet-superconductor hybrids, in particular molecules adsorbed on superconducting surfaces, in collaboration with experimental groups in Donostia and Hamburg.

We studied nonequilibrium states that appear in disordered Chern insulators after slow quenches across a topological quantum critical point. We found that the characteristic size of inhomogeneities in these states obeys the Kibble-Zurek scaling. Within the density functional theory we investigated the electrochemical degradation of electrolytes for magnesium batteries.

In the area of complex networks, we investigated hidden higher-order geometries (simplicial complexes) and their influence on the course of stochastic processes on different networks. In human brain networks created based on experimental data from the Human Connectome Project, we determined the structure of complexes attached to eight central nodes, which allow higher-order connections between different

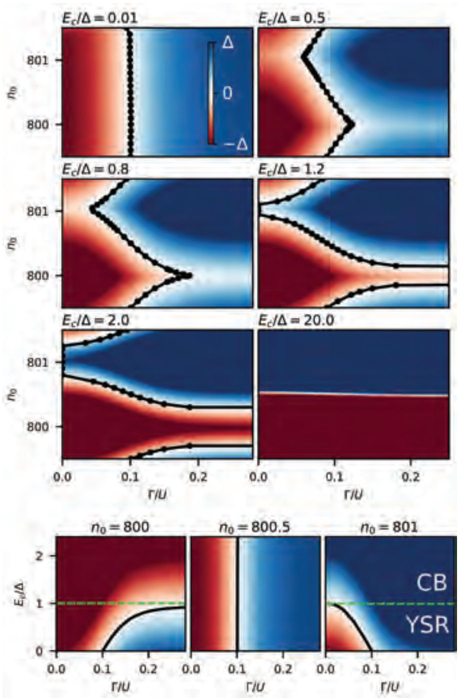


Figure 3: Transition from the regime of Yu-Shiba-Rusinov (YSR) states to the Coulomb blockade (CB) regime in the system of coupled quantum dot and ultra-small superconducting island.

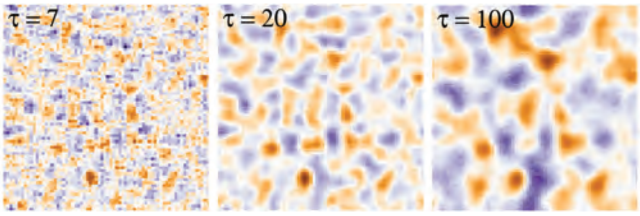


Figure 4: Post-quench profiles of the local Chern marker for different quench times τ.

brain regions. We developed a self-assembly model of preformatted groups of particles, which we describe using simplexes of a specific size and one defect connection. We showed that this process leads to a complex structure of the particle assembly with a long-range organization of defect connections. We characterized the resulting structures using the algebraic topology methods

We developed a microscopic model of the spread of SARS-CoV-2 viruses, which considers the interaction of the biological and social components of this stochastic process. Based on multiple simulations, we have analysed different types of social locking that lead to a more-or-less successful prevention of the spread of the virus.

In collaboration with the experimental group from the laboratory for calorimetry we have investigated theoretical predictions for the electro-caloric response of the lanthanum-modified lead zirconium titanate (PLZT) ceramics. We have shown that a maximum response occurs near the paraelectric to ferroelectric transition due to the presence of latent heat at the phase transition.

Some outstanding publications in the past year

1. Mierzejewski, Marcin, Vidmar, Lev. Quantitative impact of integrals of motion on the eigenstate thermalization hypothesis. *Physical review letters*, ISSN 0031-9007. [Print ed.], 2020, vol. 124, no. 4, str. 0-40603-1-040603-8, doi: 10.1103/PhysRevLett.124.040603. [COBISS.SI-ID 15846915]
2. Pourovskii, Leonid, Mravlje, Jernej, Pozzo, Mario, Alfe, D. Electronic correlations and transport in iron at Earth's core conditions. *Nature communications*. 2020, vol. 11, str. 4104-1-4105-8. ISSN 2041-1723. DOI: 10.1038/s41467-020-18003-9. [COBISS.SI-ID 50940163]
3. Ulčakar, Lara, Mravlje, Jernej, Rejec, Tomaž. Kibble-Zurek behavior in disordered Chern insulators. *Physical review letters*, ISSN 0031-9007. [Print ed.], 2020, vol. 125, iss. 21, str. 216601-1-216601-6, ilustr., doi: 10.1103/PhysRevLett.125.216601. [COBISS.SI-ID 47453187]

Awards and appointments

1. Lara Ulčakar: L'Oreal Adria and Slovene committee at Unesco award.
2. Jan Šuntajs, Prešeren Award, University of v Ljubljana, master's thesis "Spectral properties of the t-J model and many-body localization"
3. Luka Medic, Prešeren Award, University of v Ljubljana, master's thesis " Topological quantization of the transconductance in a Josephson junction with the Rashba interaction"

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

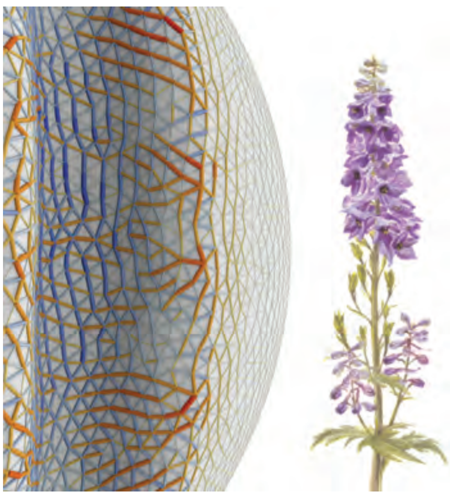


Figure 5: Inhomogeneities in the elastic properties of pollen grains determine their harmomegathic response to dehydration

We studied the role of symmetry for the stability of dipole orientations positioned on Caspar-Klug lattices, and we analysed the various aspects of electrostatic interactions between a model SARS-CoV-2 virus and a charged electret fibre. We also explored the structural stability of the SARS-CoV-2 spike protein via the mapping of the hydration free energy by the Poisson–Boltzmann method, and we theoretically investigated the gain in nanomechanical stability of this protein compared to SARS-CoV from 2002. We wrote a review focused on the role of relative humidity in the droplet spread of illnesses. By combining molecular dynamics simulations and kinetic modelling, we investigated the stability of biological fluids under negative-pressure conditions encountered in plants. Our findings show that the presence of lipid aggregates imposes an upper limit for the magnitude of the negative pressure, thereby restricting the height to which trees can grow. We explored the role of elastic inhomogeneities in pollen folding, showing how different designs of pollen grains lead to different harmomegathic responses.

We studied the active mechanics of cell-cell junctions in epithelial tissues and we found that active tension fluctuations at the junctions fluidize the tissue, which can have major implications for the overall three-dimensional tissue shape. By theoretically exploring the shapes of model active organoids, we showed that these artificial tissue-like entities can form a range of complex morphologies including the often observed branched shape. We proposed a theoretical framework that couples a vertex model of solid confluent tissues with the dynamics describing the generation of local force dipoles in the junctional actomyosin. We also studied why the skin epithelium deforms differently in cases of the basal and squamous cell carcinoma, which have very different prognoses. We found that this happens because of the differential mechanical properties of the extracellular matrix secreted by the cancer cells. Also explored in detail were the shapes of vesicle doublets. Based on experiments we proposed a model where the surface tensions of the contact and the non-contact parts of the membrane are different.

We studied the structure in 3D liquid-crystalline phases with continuous grids. We proposed the arrangement of achiral molecules in chiral cubic phases and modelled the resonant X-ray scattering response that can be expected for such a structure. We wrote a review article on the use of the resonant X-ray scattering to detect chiral structures in liquid crystals in which the constituent molecules are achiral. Also studied theoretically were 2D quasicrystals formed by clusters of bosons and marked by small, yet finite superfluidity.

- **Lipid bilayers impose a strict limit of negative pressures in biological liquids**
- **We discovered that the malignancy of different types of skin cancers depends on the mechanical properties of the extracellular matrix.**

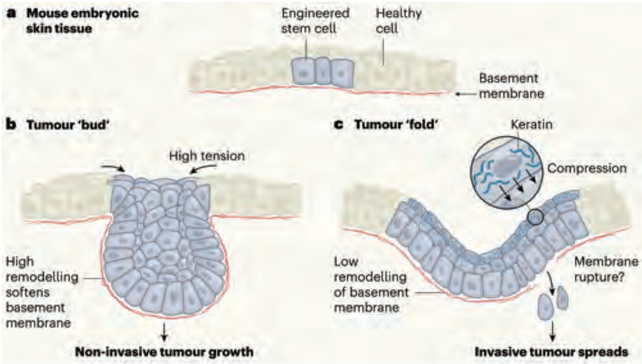


Figure 6: Basal cell carcinoma and squamous cell carcinoma differ in the mechanical properties of the extracellular matrix

Some outstanding publications in the past year

1. Fiore, V., Krajnc, M., Quiroz, F. G., J. Levorse, J., Pasolli, H. A., Shvartsman, S. Y. And E. Fuchs, E., *Mechanics of a multilayer epithelium instruct tumor architecture and function, Nature* **585**, 355 (2020).
2. Rozman, Jan, Krajnc, Matej, Ziherl, Primož. Collective cell mechanics of epithelial shells with organoid-like morphologies. *Nature communications*, ISSN 2041-1723, July 2020, vol. 11, art. no. 3805, 9 str., ilustr., doi: 10.1038/s41467-020-17535-4. [COBISS.SI-ID 24820483]
3. Lošdorfer Božič, Anže, Šiber, Antonio. Mechanical design of apertures and the infolding of pollen grain. *Proceedings of the National Academy of Sciences of the United States of America*, ISSN 0027-8424, [in press] 2020, 8 str., doi: 10.1073/pnas.2011084117. [COBISS.SI-ID 31841795]
4. Kanduč, Matej, Schneck, Emanuel, Loche, Philip, Jansen, Steven, Schenk, H. Jochen, Netz, Roland R. Cavitation in lipid bilayers poses strict negative pressure stability limit in biological liquids. *Proceedings of the National Academy of Sciences of the United States of America*, ISSN 1091-6490. [Online ed.], 2020, vol. 117, no. 20, str. 10733-10739, doi: 10.1073/pnas.1917195117. [COBISS.SI-ID 13623043]

Awards and appointments

1. Prof. Dr Jernej Fesel Kamenik, Robert Blinc award for physicists at the start of their career, Faculty of Mathematics and Physics, University of Ljubljana
2. Lara Ulčakar: L'Oreal Adria and Slovene committee at UNESCO award.
3. Jan Šuntajs, Prešeren Award, University of v Ljubljana, master's thesis "Spectral properties of the t-J model and many-body localization"
4. Luka Medic, Prešeren Award, University of v Ljubljana, master's thesis

Organization of conferences, congresses and meetings

1. Nonequilibrium quantum workshop: Nonequilibrium dynamics and ergodicity in complex quantum systems, Krvavec, 14.-17. 12. 2020 (virtual)

INTERNATIONAL PROJECTS

1. COST CA15108; Connecting Insights in Fundamental Physics (FUNDAMENTALCONNECTIONS)
   Prof. Jernej Fesel Kamenik
   Cost Office
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. The Flavor of the Invisible Universe
   Asst. Prof. Nejc Košnik
   Slovenian Research Agency
5. New Searches for Physics Beyond the Standard Model
   Prof. Jernej Fesel Kamenik
   Slovenian Research Agency
6. Manifestation of Quantum Chaos in Quantum Many-Body Lattice Systems
   Asst. Prof. Lev Vidmar
   Slovenian Research Agency
7. 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. New physics implications of scalar resonances at the LHC
   Prof. Jernej Fesel Kamenik
3. High-resolution optical magnetometry with cold cesium atoms
   Prof. Rok Žitko
4. Slow thermalization in quantum many-body systems
   Prof. Peter Prelovšek
5. Diagnosing nonequilibrium quantum matter
   Asst. Prof. Lev Vidmar
6. The influence of additives on nanoscopic wetting
   Dr. Matej Kanduč
7. Multi-scale modeling of non-equilibrium quantum materials
   Dr. Denis Golež
8. Three advances towards realistic description of strongly correlated electron transport
   Asst. Prof. Jernej Mravlje
9. Symmetries and quantum pumping
   Dr. Zala Lenarčič

VISITORS FROM ABROAD

1. Dr Sophie Renner, SISSA, Trieste, Italy, 22.-24. 1. 2020
2. Dr Manuel Szewc, International Center for Advanced Studies (ICAS) UNSAM, Buenos Aires, Argentina, 23.-28. 2. 2020
3. Toshikaze Chiba, Tohoku University, Sendai, Japan, 1.-30. 3. 2020
4. Dr Darius Faroughy, University of Zürich, Switzerland, 4.-6. 3. 2020
5. Prof. Dr Ilja Doršner, University of Split, Faculty of Electrical Engineering, Mechanical Engineering and Naval Architecture, Split, Croatia, 4.-21. 3. in 5. 7.-5. 9. 2020
6. Prof. Dr David Weiss, The Pennsylvania State University, University Park, Pennsylvania, USA, 22.-28. 3. 2020
7. Dr Roman Rausch, Kyoto University, Kyoto, Japan, 8.-12. 3. 2020
8. Dr Michele Tammaro, University of Cincinnati, USA, 26. 8. – 30. 9. 2020
9. Dr Lorenzo Ubaldi, SISSA, Trieste, Italy, 10.-13. 9. 2020

STAFF

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1. Prof. Borut Bajc
2. Prof. Janez Bonča*
3. Prof. Mojca Čepič*
4. *Dr. Barry Michael Dillon, left 01.10.20*
5. Prof. Svjetlana Fajfer
6. **Prof. Jernej Fesel Kamenik, Head**
7. Dr. Denis Golež
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9. Asst. Prof. Jure Kokalj*
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12. Dr. Zala Lenarčič
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27. Prof. Rok Žitko

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29. *Dr. Friedrich Johannes Krien, left 01.07.20*
30. Patrycja Katarzyna Lydzba, B. Sc.
31. Clement Adrien Zankoc, B. Sc.

Postgraduates

32. Blaž Bortolato, B. Sc.
33. Victor Francisco Guada Escalona, B. Sc.
34. Arman Korajac, B. Sc.
35. Luka Medic, B. Sc.
36. Luka Pavešić, B. Sc.
37. Jan Rozman, B. Sc.
38. Urša Skerbiš Štok, B. Sc.
39. Aleks Smolkovič, B. Sc.
40. Marin Šako, B. Sc.
41. Jan Šuntajs, B. Sc.
42. Martin Ulaga, B. Sc.
43. *Lara Ulčakar, B. Sc., left 01.12.20*

Technical officers

44. Miha Mohorčič, B. Sc.

Technical and administrative staff

45. Nevenka Hauschild

Note:

* part-time JSI member

BIBLIOGRAPHY

Original Article

1. Arturo Moncho-Jorda, Ana B. Jódar-Reyes, Matej Kanduč, Alicia Germán-Bellod, Alicia López-Romero, Rafael Contreras-Cáceres, Francisco Sarabia, Miguel García-Castro, Héctor A. Pérez-Ramírez, Odriozola Gerardo, "Scaling laws in the diffusive release of neutral cargo from hollow hydrogel nanoparticles: paclitaxel-loaded poly(4-vinylpyridine)", *ACS nano*, 2020, **14**, 11, 15227-15240.
2. Wiktor Lewandowski, Nataša Vaupotič, Damian Pociecha, Ewa Górecka, Luis M. Liz-Marzán, "Chirality of liquid crystals formed from achiral molecules revealed by resonant X-ray scattering", *Advanced materials*, 2020, **32**, 41, 1905591.
3. Evgeny Z. Liverts, Rajmund Krivec, Nir Barnea, "Collinear configuration of the helium atom and two-electron ions", *Annals of physics*, 2020, **422**, 168306.

4. Clément Zankoc, Matej Krajnc, "Elasticity, stability, and quasioscillations of cell-cell junctions in solid confluent Epithelia", *Biophysical journal*, 2020, **119**, 9, 1706-1711.
5. Kei Murakami, Ryuta Ebihara, Takuma Kono, Toshikaze Chiba, Yuka Sakuma, Primož Ziherl, Masayuki Imai, "Morphologies of vesicle doublets: competition among bending elasticity, surface tension, and adhesion", *Biophysical journal*, 2020, **119**, 9, 1735-1748.
6. Victor Guada, Miha Nemevšek, Matevž Pintar, "FindBounce: package for multi-field bounce actions", *Computer physics communications*, 2020, **256**, 107480.
7. Michael Schüler, Denis Golež, Yuta Murakami, Nikolaj Bittner, Andreas Hermann, Hugo U. R. Strand, Philipp Werner, Martin Eckstein, "NESSi: The Non-Equilibrium Systems Simulation package", *Computer physics communications*, 2020, **257**, 107484.
8. Bosiljka Tadić, Miroslav Andjelković, Milovan Šuvakov, Geoff J. Rodgers, "Magnetisation processes in geometrically frustrated spin networks with self-assembled cliques", *Entropy*, 2020, **22**, 3, 336.
9. Ilja Doršner, Svjetlana Fajfer, Monalisa Patra, "A comparative study of the S_1 and U_1 leptoquark effects in the light quark regime", *The European physical journal. C*, 2020, **80**, 204.
10. Damir Bečirević, Svjetlana Fajfer, Nejc Košnik, Aleks Smolkovič, "Enhanced CP asymmetries in $B \to K\mu^+\mu^-$", *European physical journal. C, Particles and fields.*, 2020, **80**, 940.
11. Philipp Terhörst, Kevin Riehl, Naser Damer, Peter Rot, Blaž Bortolato, Florian Kirchbuchner, Vitomir Štruc, Arjan Kuijper, "PE-MIU: a training-free privacy-enhancing face recognition approach based on minimum information units", *IEEE access*, 2020, **8**, 93635-93647.
12. Matej Pavšič, "On negative energies, strings, branes, and braneworlds: a review of novel approaches", *International journal of modern physics A*, 2020, **35**, 33, 2030020.
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Scientific Monograph

1. Matej Pavšič, *Stumbling blocks against unification: on some persistent misconceptions in physics*, World Scientific, 2020.

University, Higher Education or Higher Vocational Education Textbook

1. Simon Čopar, Daniel Svenšek, Aleš Mohorič, Saša Prelovšek, *Rešene kolokvijske naloge iz klasične fizike*, Fakulteta za matematiko in fiziko, 2020.
2. Andrej Zorko, Miha Nemevšek, Nejc Košnik, Matic Lubej, *Rešene naloge iz moderne fizike*, Fakulteta za matematiko in fiziko, 2020.

Theses and Mentoring

1. Daniel Dziob, *Researching innovative strategies for enhancement of understanding and motivation in science:* doctoral dissertation, Ljubljana, 2020 (mentor Mojca Čepič; co-mentor Dagmara Sokołowska).
2. Lara Ulčakar, *Non-equilibrium dynamics of topological insulators:* doctoral dissertation, Ljubljana, 2020 (mentor Tomaž Rejec; co-mentor Jernej Mravlje).

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 of atomic, molecular, optical and nuclear physics. A deep understanding of atomic and nuclear processes is paramount for the interdisciplinary research conducted at our department, which 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. In addition, our researchers are among the regular users of large research facilities worldwide, such as particle accelerators, synchrotrons and free-electron lasers. These facilities are accessed either through self-initiated applications or through international collaborations and research networks. To counterweight this process, access to the beamtime at the JSI tandem ion accelerator is available for international users within the EU H2020 project RADIATE.

Head:
Prof. Primož Pelicon

We have continued our work at the three-spectrometer facility of the Mainz Microtron (MAMI), with the focus on analysing and publishing the results on the data acquired during recent production runs. Our measurements of the polarization transfer in proton knock-out from carbon nuclei have been published (*Brecelj et al, Phys. Rev C 2020*), accompanied by a detailed study of the induced polarization component in general A(e,e'p) processes in non-coplanar kinematics (*Paul et al., Phys. Lett. B 2020*). While the study by *Brecelj et al.* was aimed at the issue of "universality" in the proton elastic form-factor ratios for various nuclei, which is related to the possible modification of the form-factors of embedded protons, we have also examined the effect of local nuclear density by investigating the polarization-transfer to protons bound in different (s and p) shells of the carbon nucleus (*Kolar et al., Phys. Lett. B 2020*). We have (re)analysed the elastic electron scattering on protons for very low-momentum transfer (data acquired in the ISR experiment) and studied the role of specific models in the extraction of the proton radius (*Mihovilovič at al., Frontiers in Phys. 2020*), a persistently elusive quantity constituting the so-called "proton radius puzzle". As part of our MAGIX Collaboration involvement, we studied the response of Cherenkov radiators for calorimetry in the energy range below 14 MeV (*Christmann et al., Nucl. Instr. Meth. A 2020*).

Our work at the Thomas Jefferson National Accelerator Facility (Jefferson Lab) has also been focused on the analysis of data from several experiments performed during the 6-GeV CEBAF era. One of the most resounding results of our measurements of deeply virtual Compton scattering off the neutron was the flavour separation of helicity-conserved Compton form-factors, which has now been published in Nature Physics (*Benali et al., Nature Physics 2020*). We have continued to analyse the data from a comprehensive group of experiments using the tritium target, which offers a unique opportunity to explore ^{3}H and its mirror nucleus, ^{3}He, and allows us to assess the validity of crucial model assumptions, in particular the isospin symmetry. The results of our measurement of the ^{3}He spin-structure functions and of neutron spin-dependent sum rules at low momentum transfers have also been published (*Sulkosky et al., Phys. Lett. B 2020*). The analysis of the experiment probing few-body nuclear dynamics by measuring ^{3}H(e,e'p)pn and ^{3}He(e,e'p)pn cross-sections at large momentum transfers and xBj > 1 has also been finished and published (*Cruz-Torres et al., Phys. Rev. Lett. 2020*). Finally, we have completed the analysis of our measurement of inclusive cross-section from 48Ca and 40Ca isotopes *(Nguyen et al., Phys. Rev. C 2020)*: by comparing the xBj-dependence of the cross-sections from ^{48}Ca to those from ^{40}Ca in a kinematic region dominated by short-range correlations (SRCs) we have provided a new way to study the isospin structure of SRCs in Ca isotopes.

Figure 1: New hypersonic jet target at the A1 experimental hall in Mainz Microtron (MAMI), built for an upcoming series of high-precision nuclear experiments with electrons on various nuclear targets.

The biggest event in the Nuclear Astrophysics Laboratory in 2020 was the approval and start of the H2020 EU project CleanHME (Clean Hydrogen Metal Energy), where JSI is collaborating with 14 consortium members in the field of research and applications of nuclear reactions based on hydrogen-metal and plasma systems. The project has started with great enthusiasm, and the kick-off meeting was held at the University of Szczecin on September 23-25, 2020.

In parallel with the construction of the FAIR (Facility for Anti-proton 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 (Darmstadt, Germany) premises. Our primary focus here is the NUSTAR physics programme devoted to nuclear structure, reactions and astrophysics, crucial for understanding the creation of all the matter in the universe, specifically in High-Resolution In-Flight Spectroscopy/ Decay Spectroscopy (HiSpec/DeSpec), Super Fragment Separator (SuperFRS) sub-collaborations. HiSpec/DeSpec experiments aim to address the key issues in nuclear structure, reactions and nuclear astrophysics at the limits of nuclear existence. A key veto system based on BGO (bismuth germanate) detectors was further optimized by our group, including the optical transport simulations, development of readout electronics and photodiode placement optimization. We have been actively involved in the first H/D Phase 0 experiment in which the structure of the heaviest $N=Z$ nuclei was studied. We have also been involved in the instrumental build-up of HISPEC-10, aimed at an investigation of short-lived or chemically inert nuclei. The main instrument of the NUSTAR collaboration is the Fragment Separator (FRS), to be superseded by a more capable SFRS, designed to be the only magnetic separator in the world capable of separating intense beams of ions of any element, up to uranium. The mass selectivity of the (S)FRS is further drastically improved with a TOF mass separator – for the latter, we have previously developed an electrostatic lens-stabilization monitor and after the installation achieved the world record in mass resolution of TOF spectrometers. We have participated in experiments measuring the masses of ground states of Pd-63 and As-69 as well as in experiments studying the exotic decay of Br-69 and Rb-73. We have also been involved in a new isotope search in the Pb-208 region experiments for FAIR phase-0 programme with stopped FRS beams. For the R3B collaboration, we have assembled and characterised 60 detector elements for the CALIFA scintillation calorimeter.

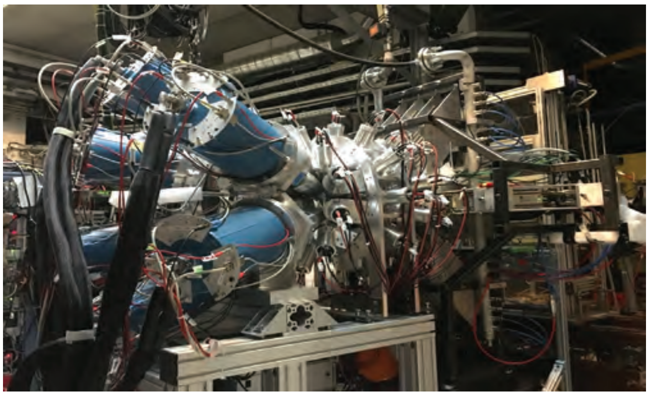

Figure 2: DeSpec setup at FAIR for 2019/2020 experimental campaign

Members of the Ionizing Radiation Measurements Group were involved in research activities related to the ionising radiation monitoring and nuclear physics. In addition, they conducted the environmental radioactivity monitoring of the living environment in Slovenia, regular Krško Nuclear Power Plant (KNPP) off-site environmental radioactivity monitoring, independent verification of the regular environmental radioactivity monitoring around KNPP, monitoring of the radioactivity in fodder, central radioactive waste repository radiological monitoring, monitoring of the radioactivity in drinking water, material characterizations, calibrations of the radiation gauges and the measurements of the personal and environmental doses by thermo-luminescent dosimeters. These activities are accredited according to the SIST EN ISO/IEC 17025 standard. Our results at the international intercomparisons regularly rank among the best of the participating institutions. Based on this performance, we are often invited to collaborate in groups for the characterization of reference materials. In 2020, together with a Scottish-Austrian partner, we prepared 460 samples in 89 sets for four international intercomparisons. The samples were characterized and tested in accordance with the requirements of international standards. A total of 62 laboratories from 14 countries from five continents participated in these intercomparisons.

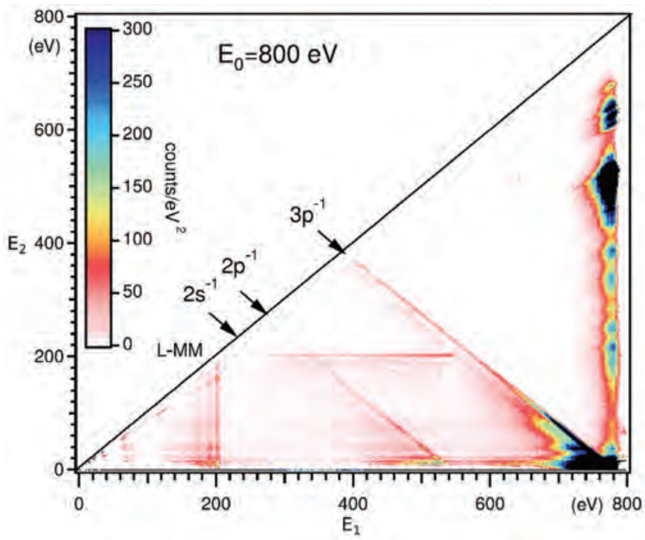

Figure 3: Measured frequency distribution of electron pairs with energies E_1 and E_2 emitted by argon atoms when bombarded with electrons of 0.8 keV initial kinetic energy (Ž. Barba et al., Rev, Sci. Instrum. 91, 073108 (2020)).

As a designated institution and as the holder of the national standard for ionizing radiation, we continued the activities on the projects from the EU EMRP project: "Preparedness – Metrology for mobile detection of ionising radiation following a nuclear or radiological incident". In collaboration with UPC, Barcelona, Spain, we were developing and upgrading a novel gamma-radiation hotspot locator with an angular sensitivity to operate on an unmanned helicopter. In 2020 we started the sampling and analysis of groundwater, thermal waters, precipitation and surface water in the area of influence of 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 purpose of the project is to determine the state of the environment before the start of the construction of HPP Mokrice. Our group participates in the task of determining the concentration activities of ^{3}H and the total content of alpha and beta emitters in water from boreholes in the construction area of the HPP Mokrice.

We continued with the study of the presence of organically bound tritium (OBT) and ^{14}C in various terrestrial and aquatic biota in the vicinity of the Krško NPP and at reference locations. In 2020 we replaced radioactive sources in the NDS, ^{137}Cs (July 22, 2020) and ^{60}Co (October 21, 2020). With the new sources we increased the field strength of ionizing radiation at ^{137}Cs by 5 and at ^{60}Co by a factor of 30.

In 2020 we successfully completed the ENRAS (Ensuring the safety of intervention teams in the event of nuclear or radiological accidents) project within the Crossborder Cooperation Program Interreg V-A Slovenia–Croatia 2014–2020. The project involves JSI as a leading partner, the Institute for Medical Research and Occupational Medicine - IMI from Zagreb, and the Firefighting Association of Slovenia. The purpose of the project was to develop a cross-border cooperation in ensuring the safety and competence of civil protection in the event of a nuclear or radiological accident. In the framework of the project, we trained a total of 800 firefighters in Slovenia and Croatia in individual trainings. Moreover, 290 firefighters from both sides of the border took part at 9 joint exercises. Thus, we realized all the goals of the project and laid the foundations for further education and training of intervention workers in the Republic of Slovenia.

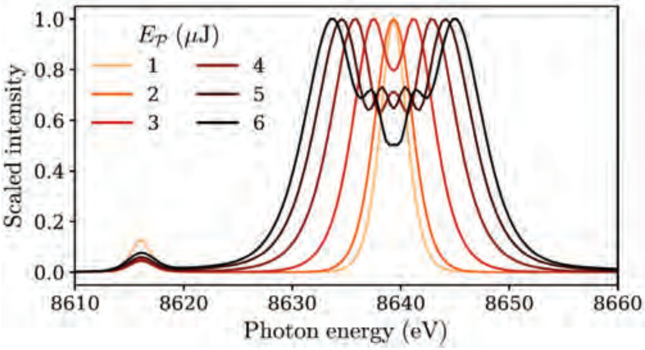

Figure 4: Calculated spectral intensity of radiation emitted in the direction of the incident light beam by a 5-μm-long zinc target at the transitions Kα1 (~8639 eV) and Kα2 (~8616 eV) at different energies of the probe light pulse. At high light intensities, the calculation predicts the Autler-Townes split of self-triggered stimulated emission Kα1 (Š. Krušič et al., PRA 102, 013102 (2020)).

In the research field of atomic and molecular physics, we completed the development of a unique instrument for electronic gas scattering research in our home laboratory. The magnetic bottle spectrometer was coupled to a pulsed source of electrons and its operation was demonstrated by measuring the scattering of electrons with a kinetic energy of 0.8 keV on argon. We measured the energy distribution of the electron pairs created by the electron ionization of the outer shells of the atom *(Barba et al., Rev, Sci. Instrum. 2020)*. The manufactured electron-driven magnetic bottle spectrometer allows the detection of a large number of electrons emitted by atoms due to electron scattering and offers parallel measurements of many decay channels with unprecedented efficiency.

In 2020 we published several research results obtained with synchrotron light. With two holes in different atomic shells, the deeper hole usually decays first, unless the outer hole decays with an ultrafast Coster-Kronig decay. We studied the decay of the $1s2s2p^6(3s/3p)$ state in Ne^+ ions, for which there is competition between the 1s and 2s core-hole decay, in collaboration with French researchers on the Soleil synchrotron. From the electronic spectra recorded with a magnetic bottle spectrometer, we determined the ratio of the two decay paths *(Jänkälä et al., Phys. Rev. A 2020)*. Synchrotron light was also used to observe single-photon absorption in benzene, where, along with the ionization of the molecule (an electron is ejected from the K shell on a carbon atom), an additional excitation of the second electron occurs, leading to the so-called K-2V molecular states. Auger spectra recorded with a magnetic bottle have a rich structure, which was explained by the DFT and Hartee-Fock calculations (*Carniato et al., J. Phys. B: At. Mol. Opt. Phys. 2020)*. In collaboration with our colleagues, we published the most accurately measured Auger spectra of KLL to date; the Auger electrons are emitted by argon atoms after K-shell ionization with synchrotron light. The experimental results are accompanied by a detailed analysis of the measured spectra, where we contributed a part of the calculations. The measurements were performed at two photon energies (3216 eV and 3400 eV), so that in the analysis, it was possible to distinguish between the Auger spectra emitted by satellite states in the preparation of the initial state with a K-shell hole and the shake-up contributions that occur due to the Auger decay of a simple K hole *(Püttner et al., Phys. Rev. A 2020)*.

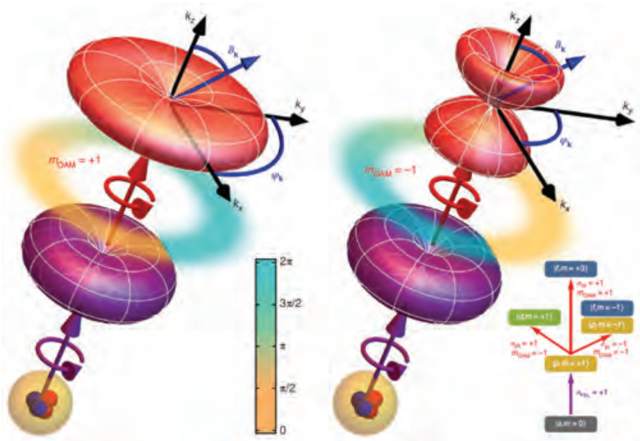

Figure 5: Predicted change in the angular distribution of the photoelectron after absorption of a photon from a stream of infrared light with an orbital angular momentum (OAM) of +1 or -1 (red arrow). The helium atom from which the photoelectron originates is located in the vertex of the light beam. Primary ionization is caused by a photon from a circularly polarized VUV light pulse generated by a free-electron laser (purple arrow). The effect observed in the experiment is not so pronounced due to the spatial smearing of the helium gas target (G. De Ninno et al., Nature Photonics 14, 554 (2020)).

In the field of theoretical atomic and molecular physics dealing with laser light in the XUV and X-ray wavelength regions, we improved the modelling of self-triggered stimulated emission. One of the problems in a conventional process simulation with Maxwell-Bloch equations is the correct treatment of spontaneous emission. We calculated the Zn-Kα emission spectrum using quantum correlation functions to describe spontaneous emission in the first part of the propagation, and the usual approach in the second part, where the spontaneous contribution becomes negligible with respect to the stimulated radiation. In the publication, we predict the Autler-Townes splitting of the spectral line after excitation by attosecond pulses of strong light recently

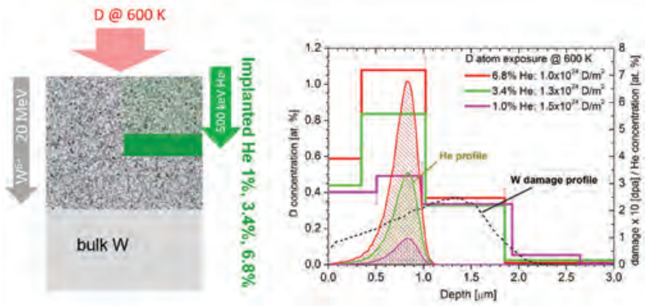

Figure 7: Left: the scheme of the W/He irradiation and D exposure procedure on W samples. The samples were exposed to a thermal deuterium (D) atom beam at 600 K to populate all the created defects. Right: the D depth profiles as measured at the end of the D exposure. The hashed area shows the He implantation depth profile and the dashed line shows the W ion damaged profile, both calculated with the binary collision program SRIM. The D concentration is the highest where the maximum He concentration is anticipated, and increases with the He concentration (Markelj et al. Nucl. Fusion 60 (2020) 106029).

generated by a free-electron laser LCLS *(Krušič et al., Phys. Rev. A 2020)*. It is known that photons carry a limited spin angular momentum, but it is less known that a photon beam can also have an unlimited orbital angular momentum. The latter depends on the azimuthal dependence of the phase of the electromagnetic wave in the plane transverse to the direction of the wave's propagation. In the paraxial approximation, both types of angular momenta are well defined. In collaboration with researchers from the University of Nova Gorica, we were able to show by measuring dichroism that the orbital angular momentum from a twisted beam of IR light can be transferred to a single electron emitted by an atom during ionization with circularly polarized XUV light *(De Ninno et al., Nature Phot. 2020)*. The finding may be technologically important because it allows the controlled formation of short-term and localized magnetic fields. In 2020 we also completed and published an analysis of time-sensitive measurements of fluorescence spectra emitted by a helium atom in the 1s3p → 1s2s transition. The 1s3p initial state excitation occurred with a fs light pulse on the FERMI free-electron laser source in a well-defined instant, and time dependence of the fluorescence line intensity was measured by a "streak" camera that detects photons with a time resolution of a few ps. An undulation of the fluorescence signal resulting from the Zeeman splitting of the initial states in a strong magnetic field was observed. The field was due to the strong permanent magnet close to the target that is required to operate the magnetic bottle spectrometer *(LaForge et al., J. Phys. B: At. Mol. Opt. Phys. 2020)*. We have devised an advanced theoretical approach for the calculation of multiphoton ionization amplitudes and cross-sections of atoms and simple molecules (*Mihelič and Horvat, accepted for publ. In Phys. Rev. A*). The approach is based on the method of exterior complex scaling (ECS) and allows for a reliable extraction of ionization amplitudes from the region of space that is unaffected by the complex coordinate transformation. Our approach circumvents the difficulties encountered with the calculation schemes based on the projection on the complex scaled channel wave functions, numerical extrapolation of the size of the simulation volume or numerical extrapolation of regularization parameters, and thus simplifies the theoretical description of resonant processes, such as resonance-enhanced multiphoton ionization or doubly-resonant two-photon ionization.

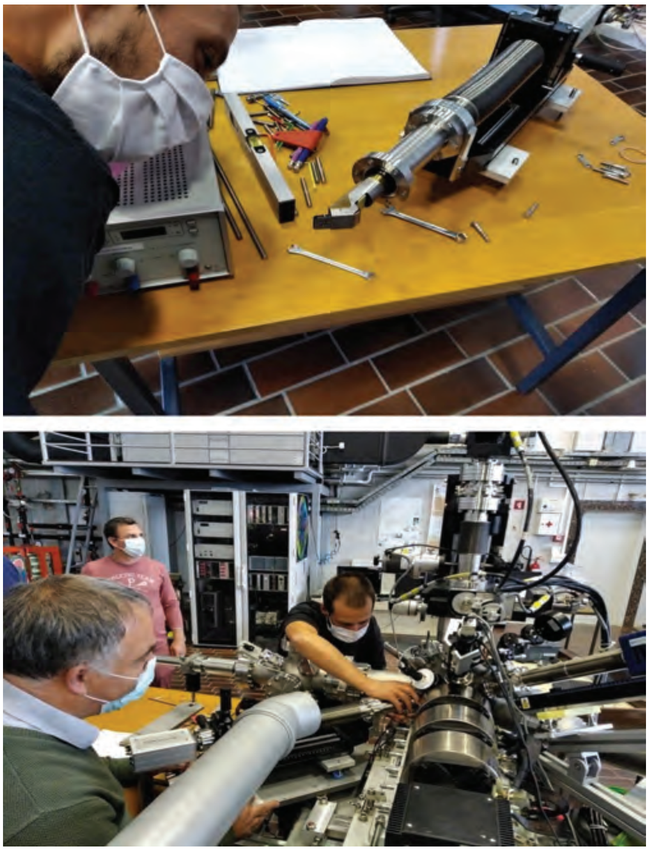

Figure 6: Installation of a new Silicon Drift Detector for the detection of characteristic X-rays in micro-PIXE spectroscopy at the JSI accelerator laboratory. The four segments of the detector configured in an annular geometry cover an extremely large detection solid angle of 1 steradian.

Mössbauer spectroscopy supported with XRD, SEM, TEM, NMR, SQUID, EPR, and EXAFS, was used to investigate the material properties of different classes of magnetic nanoparticles, environmental samples and catalysts. We contributed to the understanding of the $\alpha \rightarrow \varepsilon$ Fe_2O_3 transformation *(Tadić et al., Acta Mat. 2020)* in terms of an increased surface energy of the hollow hematite nanoparticles with a very high surface area. Therefore, taking into consideration the large surface area of the hollow nanoparticles, the α-Fe_2O_3 becomes a thermodynamically unstable phase. We demonstrated the formation and stabilization of ε-Fe_2O_3 nanostructures with an anisotropic shape and high coercivity ~20 kOe, which is one of the key properties for high-density, magnetic memory media and storage.

The influence of Fe loading in Cu–Fe catalyst material phases and its effect on carbon monoxide (CO) oxidation in H_2-rich reactant streams were investigated *(Dasireddy et al., RSC advances 2020)*. There was no change in the oxidation state of the Fe ions with copper or iron loading. In addition to the formation of the $CuFe_2O_4$ phase, the Fe and Cu were found to be incorporated into a Cu–Fe supersaturated solid solution that improved CO oxidation activity, with carbon dioxide and water produced selectively with high catalytic activity in depleted hydrogen streams.

We were active in high-resolution X-ray spectroscopy in the field of applied research to improve lithium-sulphur batteries. In this type of battery, sulphur is reduced during a discharge through a special mechanism in which the active material dissolves sequentially in the electrolyte and forms lithium polysulfides (Li_2S_x), where x is a function of the state of charge. From the spectroscopy of lithium polysulfide samples, we observed a pre-peak in the vicinity of the sulphur K absorption edge and confirmed the theoretical prediction that its relative yield depends on the length of the polysulfide chain *(Robba et al., J. Phys. Chem. Lett. 2020)*. In the field of X-ray spectroscopy, we also published an analysis of satellite and hyper-satellite contributions to the Kα emission line in the ionization of titanium with alpha particles with a kinetic energy of 3–5 MeV. *(Kavčič et al, Nucl. Instr. Meth. B 2020)*. These research activities were undertaken to improve the analysis of X-ray spectra acquired by an alpha beam of the APXS spectrometer operating at the Curiosity rover on Mars.

As part of the aerosol research in the European project EUMET-AEROMET, we investigated the operation of the low-cost optical aerosol sensor GP2Y1010AU0F in three different environments: a clean room, in a controlled atmosphere with a known size distribution of aerosols and in an urban environment polluted by traffic. The collected sensor data were used to predict the sensor response in real-world measurements, which was simultaneously monitored with a calibrated optical particle counter *(Bučar et al., Sensors 2020)*. This kind of research is important to determine the limits of reliability for low-cost sampling and measurement equipment that provides a great deal of data at countless measuring points in space and time in contrast to a few selected points with expensive and complicated measuring devices.

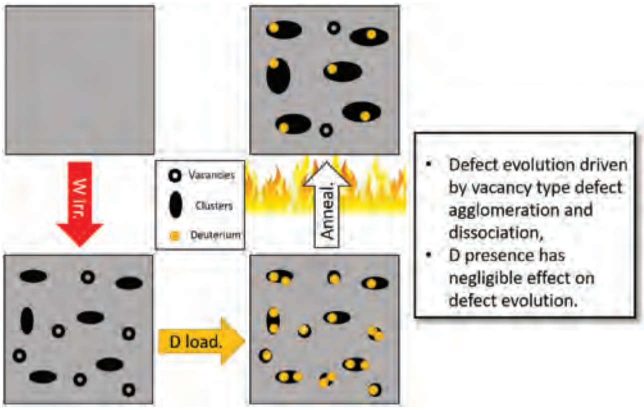

Figure 8: The procedure of the annealing experiment where W samples were first irradiated by W ions to create displacement damage, then exposed to D, annealed, and then analysed to study the presence of D on the defect evolution with the temperature. (from Pečovnik et al., Nucl. Fusion 60 (2020) 106028).

In the laboratory for fusion research coordinated by the EUROfusion Consortium within the Work Package on “Preparation of efficient Plasma-Facing Component (PFC) operation for ITER and DEMO”, we investigated the influence of helium (He) on deuterium (D) retention and transport when He is implanted inside the bulk of tungsten (W). In future fusion devices, He will be produced directly through the deuterium-tritium fusion reaction, by nuclear reactions between the wall material and neutrons and indirectly by tritium decay. For this purpose, it is important to know how He can influence the hydrogen isotope retention in future devices. The study was performed in our home laboratory where we followed the dynamics of D uptake by measuring the D depth profiles in situ during and after D exposure by nuclear reaction analysis *(Markelj et al. Nucl. Fusion 2020)*. A peak of the D concentration was measured at the position of maximum He concentration, as shown in figure 1. We show that the D retention increases linearly with implanted He fluence following a D/He ratio of 0.29. From this study we could conclude that in the main wall of a future fusion device the effect of He will not dominate D retention in W, as the retention associated with the defects in the neutron-bombarded W will dominate. However, at high heat flux areas where the displacement damage possibly anneals out, and hence the defect concentration drops, He could accumulate in the material and the He-associated retention prevails.

In the second study the effect of D on the annealing of radiation damage was addressed *(Pečovnik et al. Nucl. Fusion 2020)*. Tungsten samples were sequentially irradiated with 20-MeV W ions at room temperature and loaded with a low-temperature D plasma at 370 K to decorate the created defects. To study the evolution of the created defects with D being present, samples were annealed by heating them to a particular temperature and holding for 2 h. The surviving displacement damage was decorated by re-exposing the samples to the same D plasma as before. The schematics of the experimental procedure are shown in figure 2. We found that if there is an effect of D on the displacement damage evolution, it is very small for our chosen annealing temperatures and hold time. We have also presented a kinetic model to describe hydrogen absorption and desorption from tungsten at different surface coverages *(Hodille at el. Nucl. Fusion 2020)*. Activation energies for hydrogen absorption into the bulk and desorption from the surface of tungsten were modelled by functions that depend explicitly and continuously on the hydrogen surface coverage. With this approach we were able to successfully describe the published experimental results on the D uptake and retention of self-damaged tungsten exposed to 0.28-eV deuterium atoms at different temperatures ranging from 450 K to 1000 K, performed in our laboratory. Finally, the steady-state model was applied for extrapolation from the milder conditions in laboratory experiments to the harsh conditions present in fusion devices.

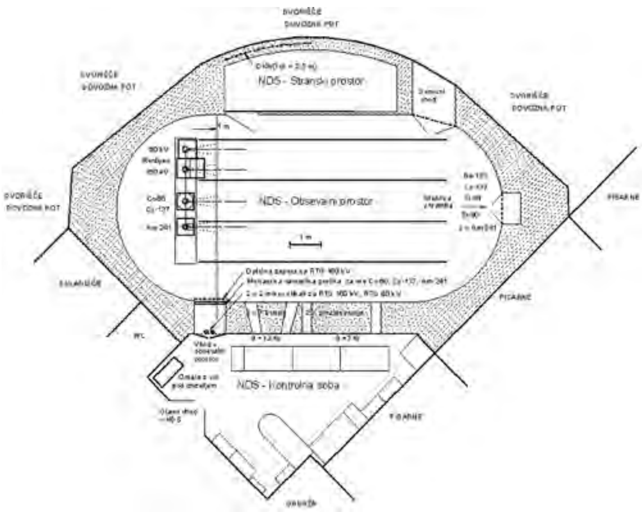

Figure 9: The National laboratory for dosimetric standards (NDS): the irradiation facility with a concrete shield and command room, providing the national etalon for ionizing radiation for the Metrology Institute of the Republic of Slovenia. New radiation sources, ^{137}Cs and ^{60}Co, were installed in 2020.

The tandem accelerator of the Jožef Stefan Institute provided 3000 beam hours to the users in 2020. We conducted extensive research with the micro-PIXE method in the field of plant biology. With collaborators from Germany, we studied the elemental distribution in developing barley grain (*Detterbeck et al. Journal of Food and Agricultural Chemistry, 2020*) and the localisation of Pb in plant leaves (*Höreth et al. New Phytologist 2020*). With collaborators from the United Kingdom, we evaluated the P distribution in roots (*Pongrac et al. BMC Plant Biology, 2020*) and gene expression in responses to the P and Zn interaction in roots (*Pongrac et al. Frontiers in Plant Science, 2020*). With collaborators from Spain, we evaluated the distribution of Al and other elements in the leaves of tea plants (*Pongrac et al. Food and Chemical Toxicology, 2020*). Within the ARRS project entitled "Ionome of crop plants for safe and quality food production", the distribution of Ca in commune bean seeds (*Cominelli et al. Food Chemistry, 2020*) and distribution and ligand environment of Fe in wheat grain (*Pongrac et al. Plants 2020*) were investigated at ESRF in Grenoble by using micro-XRF mapping and micro-XANES. At the Elettra synchrotron in Trieste we studied the distribution and ligand environment of Fe in diploid and tetraploid wheat species and the effect of Se on the uptake of Hg into the slug food chain (*Kavčič et al. Food and Chemical Toxicology 2020)*.

Figure 10: Manipulation of the new ^{137}Cs source in the hot cell of JSI. In 2020, we installed the new ^{137}Cs and ^{60}Co sources in the irradiator of the National laboratory for dosimetry standards, providing a gamma irradiation field for the national etalon of ionizing radiation.

At the ALBA synchrotron in Barcelona we used the EXAFS method to study the degradation of silver nanoparticles with PVP, citrate and PEG coatings in lettuce tissues (*Torrent et al. Journal of Hazardous Materials, 2020*). We also studied the effect of drought on the formation Ca crystals in buckwheat tissues (*Gaberščik et al., Plants, 2020*) and the effects of Si accumulation on the optical properties of leaves of *Deschampsia caespitosa* (*Grašič et al. Biologia Plantarum, 2020*).

In collaboration with the Department of Surface Technology and Optoelectronics, F4, we initiated research on the influence of low-pressure cold plasma on seed morphology, genetics and physiology *(Starič et al. Plants 2020).* In collaboration with KI we studied the parameters for distinguishing between conventional and organic chicory production (*Sinkovič et al. Food and Chemical Toxicology 2020*). In collaboration with the Department of Environmental Science (O2) we studied the geographical origin of Slovenian milk based on isotopic and elemental composition (*Potočnik et al. Food Chemistry 2020*). For the applicative project "Locally grown buckwheat grain for the production of high-quality food products" we mapped detailed tissue-specific distribution in Tartary buckwheat grain (*Pongrac et al. Fagopyrum, 2020*) and studied the connection between the nutritional quality of buckwheat and antiviral effects (*Luthar et al., Plants, 2020*).

We organised a two-day long (14th and 15th September) on-line conference ICNMTA2020 (17th International Conference on Nuclear Microprobe Technology and Applications), which attracted 151 attendees from 29 countries and six continents, who participated in the ideas exchange on recent technical advancements and the broad spectrum of focused-ion-beam applications through 21 invited talks, 26 contributed talks and 20 posters.

The high-energy focused ion (Microbeam) station was upgraded with a new and unique SDD detector that boasts four segments and offers 1 steradian of acceptance solid angle. The detector enables edge-quality quantitative elemental analysis of organic and inorganic samples in dried or frozen-hydrated state at the (sub) micron level. Thanks to its extremely large solid angle, we managed to accelerate micro-PIXE measurements by a factor of 10. The design of this detector was very demanding, as it was necessary to consider the existing geometry of the measuring chamber with respect to the ion beam: the "head" of the detector had to be bent to 45°. This challenge was taken over by the company PNDetector and the purchase of the detector was partly financed by the Public Agency for Research of the Republic of Slovenia (Public tender for co-financing the purchase of research equipment; Package 17). We continued to combine our ion microscopy work with several instrumental techniques, including the helium-ion microscope at the Helmholz Zentrum Dresden Rosendorf (HZDR) in the framework of Helmholtz European Partnering project "CROSSING", an ongoing (2019–2024) bilateral project between the JSI and HZDR involving six departments at the JSI and four institutes at HZDR.

Archaeometrical research in 2020 was again devoted to the analysis of glass; however, we now concentrated on the glass of Late Antiquity and Early Byzantine period. We competed and published a study of glass from the site Korinjski hrib from the Slovenian region Suha Krajina. During the turbulent times of the People Migration period, the site was located at the three-border point of three Roman provinces and was likely populated by a Byzantine garrison. This is reflected in the composition of the glass, which is corresponds to that in the central Balkans. The composition of the glass in this area was further investigated in a study of glass inventory from the Late Antiquity site Gradina on the Jelica Mountain in present-day Serbia. We plan a further analysis of Late Antiquity glass, which may demonstrate commercial connections in this period. We also analysed glass fragments from the Pržanj site near Ljubljana and found that most of them were late antique (Roman) natron glass, and in one case potassium glass from the modern period. The results have not yet been published.

Concerning metal analysis, we completed a comprehensive study of small Celtic coinage from Slovenia. During early work, we encountered limitations of the techniques based on irradiation with the protons, as they penetrate just a few tens of micrometres into the matter, into the region where silver alloys are typically enriched in silver. The measurements were then executed by cold neutrons at the reactor in Budapest, as the neutrons pass the whole object unscathed. So, we were able to determine the fineness of the silver through the whole coin and recognize two broad groups of coins with respect to the metal quality. This can be interpreted as two minting phases, using the metal of lower quality in the latter. We also conducted an interesting study of the authenticity of objects from the Archeo Norico Museum (otherwise privately owned). Five of the seven items turned out to be authentic or from authentic antique alloys, and two were found to be modern counterfeits.

Organization of conferences, congresses and meetings

1. ICNMTA2020, 14 –15 September 2020, on-line

Patent granted

1. Larisa Hosnar, Matjaž Vencelj, Klemen Bučar, Janez Burger, Angle-sensitive gamma camera with a rotary obstruction, GB2530574 (B), Intellectual Property Office, 02. 12. 2020.

INTERNATIONAL PROJECTS

1. CROSSING - Crossing Borders and Scales - An Interdisciplinary Approach
   Prof. Primož Pelicon
   Helmholtz-zentrum Dresden-rossendorf E.v.
2. EMPIR; Preparedness - Metrology for Mobile Detection of Ionising Radiation Following a Nuclear or Radiological Incident
   Dr. Toni Petrovič
   Euramet E.v.
3. EMPIR; AEROMET - Aerosol Metrology for Atmospheric Science and Air Quality
   Prof. Matjaž Žitnik
   Euramet E.v.
4. EMPIR - 17RPT01 DOSEtrace; Research Capabilities for Radiation Protection Dosimeters
   Denis Glavič Cindro, M. Sc.
   Euramet E.v.
5. EMPIR - supportBSS; Support for a European Metrology Network on Reliable Radiation Protection Regulation
   Denis Glavič Cindro, M. Sc.
   Euramet E.v.
6. EMPIR; AEROMET II; Advanced Aerosol Metrology for Atmospheric Science and Air Quality
   Asst. Prof. Klemen Bučar
   Euramet E.v.
7. COST CA16117 - ChETEC; Chemical Elements as Tracers of the Evolution of the Cosmos
   Prof. Matej Lipoglavšek
   Cost Office
8. 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
9. COST CA18130; European Network for Chemical Elemental Analysis by Total Reflection X-Ray Fluorescence
   Dr. Marijan Nečemer
   Cost Association Aisbl
10. COST CA18222; Attosecond Chemistry
    Asst. Prof. Andrej Mihelič
    Cost Association Aisbl
11. COST CA18212; Molecular Dynamics in the GAS Phase
    Prof. Matjaž Žitnik
    Cost Association Aisbl
12. COST CA16117; Chemical Elements as Tracers of the Evolution of the Cosmos
    Prof. Matej Lipoglavšek
    Cost Association Aisbl
13. 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
14. 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
15. 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
16. EMPIR Programme 2020 – 2027
    Denis Glavič Cindro, M. Sc.
    Clarin Eric
17. H2020 - CONCERT; European Joint Programme for the Integration of Radiation Protection Research
    Asst. Prof. Benjamin Zorko
    European Commission
18. H2020 - TRANSAT; TRANSversal Actions for Tritium
    Asst. Prof. Sabina Markelj
    European Commission
19. H2020 - RADIATE; Research and Development with Ion beams - Advancing Technology in Europe
    Prof. Matjaž Kavčič
    European Commission
20. H2020 - CleanHME; Clean Energy from Hydrogen-Metal Systems
    Prof. Matej Lipoglavšek
    European Commission
21. H2020 - EUROfusion; Plasma Facing Components-1-IPH-FU, EUROfusion
    Asst. Prof. Sabina Markelj
    European Commission
22. H2020 - EUROfusion; Education-ED-FU
    Prof. Primož Pelicon
    European Commission
23. H2020 - TissueMaps - Elemental Imaging of Human Tissue: Clinical Therapy Support and Development of New Diagnostics
    Prof. Primož Pelicon
    European Commission
24. Study of Weak Charge Distributions with Precision Parity-Violating Measurements
    Asst. Prof. Miha Mihovilovič
    Slovenian Research Agency
25. Electrochemical Reactions in Organic-Metal Batteries Studied by X-Ray Raman Spectroscopy
    Prof. Matjaž Kavčič
    Slovenian Research Agency
26. Investigation of Helium Retention in Plasma Facing Materials Using Advanced Analytical Methods
    Asst. Prof. Sabina Markelj
    Slovenian Research Agency

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. Structure of hadronic systems
   Prof. Simon Širca
4. Studies of atoms, molecules and structures by photons and particles
   Prof. Matjaž Žitnik
5. Fusion technologies
   Asst. Prof. Sabina Markelj

R & D GRANTS AND CONTRACTS

1. Triggering forbidden phenomena with twisted light and particles beams
   Prof. Matjaž Žitnik
2. Redox active organic materials for electrical energy storage
   Prof. Matjaž Kavčič
3. Ionom of crop plants for safe and quality food production
   Prof. Katarina Vogel-Mikuš
4. Stable isotopes in the study of the impact of increasing CO2 levels on C and Hg cycling in coastal waters
   Prof. Katarina Vogel-Mikuš
5. Three-dimensional distribution of mineral elements in plant leaves
   Asst. Prof. Paula Pongrac
6. Advanced surface finishing technologies for antibacterial properties of patient specific 3D printed implantable materials
   Esther Punzon Quijorna
7. Molecular imaging inside the cell
   Prof. Primož Pelicon
8. Catalysis of Nuclear Reactions by Electrons
   Prof. Matej Lipoglavšek
9. Molecular Imaging Inside the Cell
   Prof. Primož Pelicon
10. Spatial localization of elements and metabolits in plants
    Prof. Katarina Vogel-Mikuš
11. Novel proxies of the Holocene climate variability in stalagmites in Slovenia
    Prof. Primož Pelicon
12. Localy grown buckwheat grain for production of high quality food products
    Prof. Primož Pelicon
13. Innovative configuration of inductively coupled gaseous plasma sources for up-scaling to industrial-size reactors
    Dr. Marko Petric
14. Innovative ECO plasma seed treatment (for sowing and for human and animal diet/ nutrition
    Prof. Primož Pelicon
    Ministry of Education, Science and Sport
15. ENRAS: Ensuring Radiation S afety for First Responder Teams in Case of Radiological or Nuclear Accidents
    Boštjan Črnič
    Government Office for Development and European Cohesion Policy
16. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
    Prof. Primož Pelicon
    Slovenian Research Agency
17. Calibrations
    Matjaž Mihelič, M. Sc.
18. Different Analyses; Reference Materials
    Dr. Jasmina Kožar Logar
19. C-14 Measurements
    Dr. Romana Krištof

NEW CONTRACTS

1. Measurements of gaseous effluents, specific analysis of H-3 and C-14 in year 2020
   Asst. Prof. Benjamin Zorko
   Nuklearna Elektrarna Krško d. o. o.
2. Maintaining emergency preparedness and response by ELME (2020-2023)
   Asst. Prof. Benjamin Zorko
   Nuklearna Elektrarna Krško d. o. o.
3. National monitoring of radioactivity in the environment in the Republic of Slovenia for 2020
   Asst. Prof. Benjamin Zorko
   Ministry of the Environment and Spatial Planning
4. 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
   Nuklearna Elektrarna Krško d. o. o.
5. 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
   Nuklearna Elektrarna Krško d. o. o.
6. Monitoring of radioactivity in drinking water for years 2020 and 2021 (lot 2)
   Asst. Prof. Benjamin Zorko
   Ministry of Health
7. Measurements of gross alpha and beta activities in drinking water
   Dr. Jasmina Kožar Logar
   Ministry of Health
8. Qualitative and quantitative monitoring of groundwater in the impact area of the dam for HPP Mokrice
   Asst. Prof. Benjamin Zorko
   Irgo Consulting d. o. o.

VISITORS FROM ABROAD

1. Dr. Katja Magdić Košiček, IRB, Zagreb, Croatia, 1 January–15 November 2019
2. Dr. Geoffrey Grime, Univesity of Surrey, Guildford, Surrey, UK, 13–16 January 2020
3. Dr. Mira Aničić Urošević, IPB, Belgrade, Serbia, 22–28 March 2020
4. Abdulghani Shakhashiro, IAEA, Wienna, Austria, 21–23 August 2020

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6. Prof. Matjaž Kavčič
7. Dr. Jasmina Kožar Logar
8. Prof. Matej Lipoglavšek
9. Asst. Prof. Sabina Markelj
10. Asst. Prof. Andrej Mihelič
11. Asst. Prof. Miha Mihovilovič
12. Dr. Marijan Nečemer
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16. Prof. Simon Širca*
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21. Prof. Katarina Vogel-Mikuš*
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23. Prof. Matjaž Žitnik

Postdoctoral associates
24. Dr. Žiga Barba
25. *Dr. Tilen Brecelj, 20.08.20, transferred to Department E1*
26. Dr. Aleksandra Cvetinović
27. *Dr. Boštjan Jenčič, left 01.10.20*
28. Dr. Romana Krištof*
29. Dr. Eva Menart*
30. Dr. Marko Petric
31. Esther Punzon Quijorna, B. Sc.

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33. *Tim Kolar, B. Sc., left 01.10.20*
34. Gregor Košir, B. Sc.
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1. Žiga Barba, *Magnetic bottle electron spectroscopy of atomic reactions triggered by a pulsed electron beam:* doctoral dissertation, Ljubljana, 2020 (mentor Matjaž Žitnik).
2. Tim Kolar, *Measurement of recoil polarization in the* $^{12}C(\vec{e},e'\vec{p})$ *process at large virtualities:* doctoral dissertation, Ljubljana, 2020 (mentor Simon Širca).

DEPARTMENT OF THIN FILMS AND SURFACES F-3

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

Head:
Prof. Miha Čekada

For the past 10 years the department has dedicated a lot of effort to the topics of the growth defects that form in the thin films deposited by physical vapor deposition (PVD). As a resume of all these achievements, we published a review paper and a book chapter last year. They are complementary and looking from two perspectives cover all the current knowledge of growth defects in thin films. The growth defects are microstructural imperfections in a thin film having micrometre dimensions. They primarily form on spots were there are existing topographic imperfections on the substrate surface (pits, hillocks) or various foreign particles (dust, chips). The foreign particles are not only remnants of chemical cleaning, but also those that arise during heating, ion etching and film deposition. We put more emphasis on the influence of growth defects on the functional properties of thin films. The topic is relevant for all users of PVD technology, since our two works offer ways to reduce the density of growth defects, which in general decrease the quality of the deposited films.

The topic of growth defects is an interesting case of a research niche where the research work is primarily performed in industrial deposition systems, i.e., in a realistic, non-optimal environment, thus the results are directly applicable in practice. We used a similar principle in studying the non-uniformity of hard-coating thickness on geometrically irregular shapes using cathodic arc evaporation. By concentrating the electric field lines on sharp edges, such as drill corners, the thin-film deposition rate at these spots increases. This effect has been analysed in detail; we experimentally evaluated the influences of tool geometry and tool mounting type in the deposition chamber. Following these results, we optimized the deposition parameters to such an extent that the effect of coating-thickness non-uniformity was as low as possible.

We published a review paper and a book chapter, which in 80 pages provide an overview of state of the art on growth defects in thin films prepared by PVD processes.

We use various plasma diagnostic techniques to explore the physical processes in magnetron sources for the deposition of thin films. Magnetron sources can operate in DC, radio-frequency or pulsed modes. The research using high-speed cameras and other diagnostic techniques has shown that in all these magnetron regimes the plasma is concentrated in narrow areas called ionization zones. They often form periodic patterns above the magnetron cathode and have elongated shapes resembling arrows, triangles or circles. The ionization zone shape, their number, periodicity and dynamics depend on the working pressure, discharge current and cathode voltage. Using the newest high-speed camera, we made a detailed analysis of the plasma dynamics in high-power impulse magnetron sputtering. The dynamics was studied for various argon pressures, discharge currents, powers and pulsing frequencies. We found that by increasing the discharge current several periodic and aperiodic patterns appear, which change through various phases of self-organization. The ionization zones initially propagate in the opposite direction of the electron drift, but later they reverse the direction to follow the electrons. The speed of the ionization zones is 1–10 km/s.

We also studied physical processes at the atomic level that take place during the collision of an ion with matter. Using the Sigmund-Thompson analytical model of sputtering we explored the influence of several parameters on the distribution of sputtered atoms. We found that the peak of the

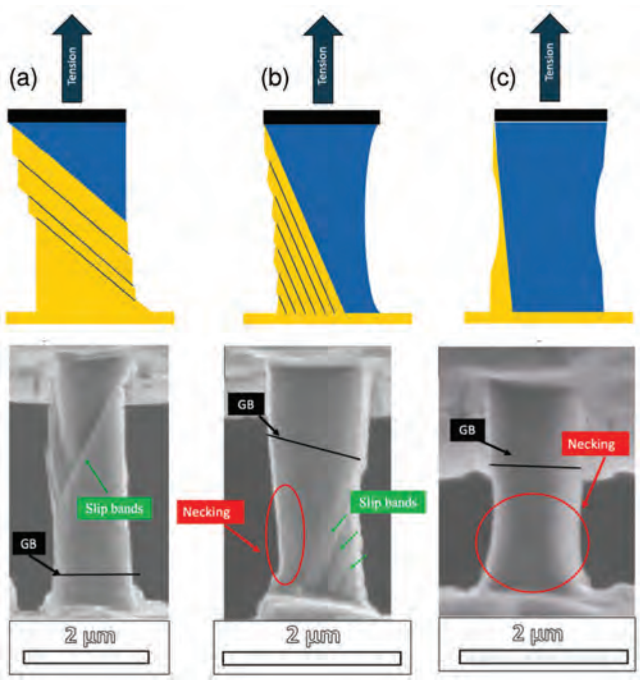

Figure 1: Tensile experiment with a nanomechanical tester; schematic overview of the (a) discrete slip mode, (b) mixed mode and (c) necking and strain hardening mode. SEM images are shown for each case too.

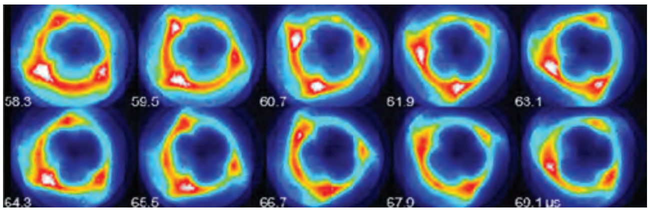

Figure 2: Dynamics of ionization zones during a pulse in high-power impulse magnetron sputtering. The images were acquired by a high-speed camera at 1.2-μs intervals.

energy distribution of sputtered atoms depends primarily on the surface binding energy of the sputtered material; we also found that the energy distribution when changing the ion mass and energy does not have such an influence in low-energy ions. The majority of high-energy atoms are sputtered by those ions that have a comparable mass to the target atoms and higher energies.

We have been collaborating with the EUROfusion programme for several years. We analyse the surface damage on tiles of the reactor's first wall, which are in contact with hot plasma. Plasma instabilities, commonly arising between the plasma and the reactor wall, can substantially damage the wall's surface. Using different techniques, we analyse morphological changes on the tungsten tiles that were exposed to plasma in the ASDEX Upgrade tokamak at the Max-Planck Institut für Plasmaphysik in Garching (Germany).

In 2019 we successfully applied for an Agency call for the co-financing of an equipment purchase; as a result we acquired last year an in-situ nanomechanical tester. The instrument is mounted in a scanning electron microscope chamber, which enables a direct observation of a nanomechanical experiment. We used a similar instrument in the scope of an informal collaboration with the Montanuniversität Leoben (Austria) and University of California, Berkeley. In the scope of this collaboration, we evaluated the trendline of fracture toughness of the CrAlN and CrAlSiN coatings up to the temperature of 700 °C in 100 °C steps. Using the in-situ nanomechanical tester we loaded each micro-cantilever up to the point of breaking. By applying the finite-element model, we determined the correct geometry and the dimensionless parameter necessary for a determination of fracture toughness. The high-temperature fracture toughness was correlated with the acquired results of high-temperature hardness and high-temperature measurements of the friction coefficient and wear. We also studied the influence of limiting/blocking on the movement of dislocations in cubic crystals during micro-tensile testing. We proposed a simple, yet effective parameter, BVR (block volume ratio), for quantifying the rate of limitation for a given slip system.

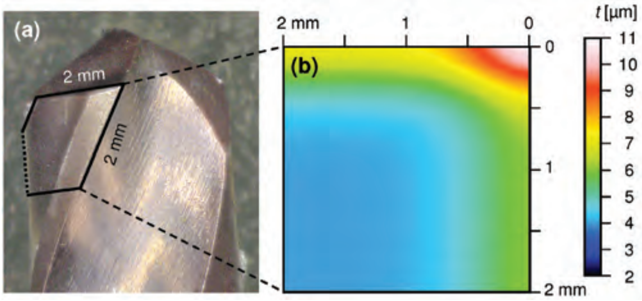

Figure 3: Modelling of the coating thickness increase, which was deposited by cathodic arc evaporation. The deposition parameters were deliberately set in a way to maximize the effect.

Several of our research topics are directed to the application of our coatings for given machining processes. Together with the Mechanical Engineering Faculty of the University of Ljubljana we evaluated the lifetime of hard coatings on tools using liquid CO_2 as a cooling medium in semi-industrial conditions. We studied the wear resistance of several coatings with an emphasis on TiAlSiN and evaluated the influence of wear and coating choice on the roughness of the machined surface. Our study showed that in addition to the cooling and lubricating conditions the choice of proper cutting parameters is important; this will be the subject of forthcoming work.

Several of these applied research topics are pursued in collaboration with partners from abroad. In collaboration with the University of Novi Sad (Serbia) we evaluated the influence of the duplex treatment (plasma nitriding and nanolayer CrAlN coating deposition) for the protection of tools for the die casting of aluminium alloys, with an emphasis on the prevention of melt sticking on the tool surface. The sticking problem was analysed for different compositions of the CrAlN coating and different tool exposure times towards the high-temperature melt. With partners from the same university, we also explored the influence of substrate materials and rotation mode during the nanolayer TiAlN/TiSiN coating deposition on the coating topography and crystal grain size. The University of Bartin (Turkey) was our partner in the optimization of coating-deposition parameters as well as the optimization of machining parameters for the milling of carbon-fibre-reinforced composites and the milling of hardened steel. The protection of cutting inserts for wood machining is the topic of joint work with the Warsaw Technical University. At the more basic-science level we collaborate with the Institute for Technical Physics and Materials Science (Hungarian Academy of Sciences) from Budapest; our task is the deposition of multilayer structures based on Si/C and W/C.

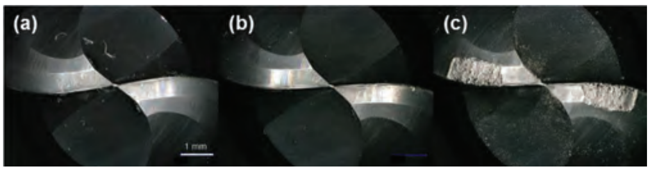

Figure 4: Wear of an endmill protected by the TiAlN coating: (a) new tool, (b) coating wear on the flank face, (c) worn tool

To a minor extent the department is also active in some other fields of coating deposition and the analytics of surfaces and thin films. In most cases the materials investigated are chemically much different than the ones from our core competence; however, our contribution is useful for other research partners who do not have the relevant instruments for this type of research. In this way we collaborate with several departments at the Jožef Stefan Institute, as well as with other research institutions, such as faculties of mechanical engineering in Ljubljana and Maribor, Faculty for natural sciences and technology at University of Ljubljana, and Institute for metals and technologies.

The collaboration with Slovenian industry takes place at several levels. The companies address us in the case of an issue connected to surfaces or thin films. This may include development projects, advanced analytics or a failure analysis. In the previous year, such analyses were performed for the companies: Balmar, Difa, Domel, Jordan, Kern, Kovinos, Le-tehnika, Mahle, Odelo, Phos, Podgorje, Proarmis and Trelleborg. Our industrial partners are also offered the service of depositing hard coatings on their tools, which we perform in the scope of our Hard Coatings Center. There are annually more than a hundred partners, which includes both large companies (e.g., Kolektor, Mahle, Hidria) as well as numerous small tool shops.

Some outstanding publications in the past year

1. P. Panjan, A. Drnovšek, P. Gselman, M. Čekada, M. Panjan, Review of growth defects in thin films prepared by PVD techniques. *Coatings*, ISSN 2079-6412, 2020, vol. 10, no. 5, pp. 447-1-447-39
2. M. Čekada, P. Panjan, A. Drnovšek, M. Panjan, P. Gselman, Growth defects in PVD hard coatings. In: Kumar, Sushil (ed.), Aswal, D. K. (ed.). Recent advances in thin films, (Materials horizons, ISSN 2524-5384). Cham: Springer. 2020, pp. 35-73

INTERNATIONAL PROJECTS

1. H2020 - EUROfusion; Plasma Facing Components-1-IPH-FU, EUROfusion
   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. Central European SME Gateway to Key-enabling Technology Infrastructures - Sparking new Transnational KET Innovation Ecosystem
   Prof. Miha Čekada
   Bay Zoltan Alkalmazott Kutatasi Kozhasznu
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. Building blocks, tools and systems for the Factories of the Future – GOSTOP
   Prof. Miha Čekada
   Ministry of Education, Science and Sport
9. Deposition of hard coatings
   Prof. Miha Čekada

VISITORS FROM ABROAD

1. Marco Beltrami, University of Trieste, Trieste, Italy, 6. 2. 2020
2. Rafko Butkovič, Vacuum-tech s.r.l., Gorizia, Italy, 26. 2. 2020
3. Rafko Butkovič, Vacuum-tech s.r.l., Gorizia, Italy, 16. 7. 2020
4. Aldo Conti, Hiden Analytical, Milano, Italy, 15. 9. 2020

STAFF

Researchers
1. **Prof. Miha Čekada, Head**
2. Dr. Aljaž Drnovšek
3. Dr. Peter Panjan
4. Dr. Matjaž Panjan

Postgraduates
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7. Uroš Stele, B. Sc.

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8. Jožko Fišer
9. Damjan Matelič
10. Andrej Mohar
11. Tomaž Sirnik
12. Tadej Stele

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Original Article

1. Peter Rodič, Barbara Kapun, Matjaž Panjan, Ingrid Milošev, "Easy and fast fabrication of self-cleaning and anti-icing perfluoroalkyl silane film on aluminium", *Coatings*, 2020, **10**, 3, 234.
2. Pal Terek, Lazar Kovačević, Aleksandar Miletić, Branko Škorić, Janez Kovač, Aljaž Drnovšek, "Metallurgical soldering of duplex CrN coating in contact with aluminum alloy", *Coatings*, 2020, **10**, 3, 303.
3. Dervis Ozkan, Peter Panjan, Mustafa Sabri Gök, Abdullah Cahit Karaoğlanli, "Experimental study on tool wear and delamination in milling CFRPs with TiAlN- and TiN-coated tools", *Coatings*, 2020, **10**, 7, 623.
4. Pal Terek, Dragan Kukuruzović, Lazar Kovačević, Aleksandar Miletić, Vladimir Terek, Branko Škorić, Peter Panjan, Miha Čekada, "The Influence of CrAlN coating chemical composition on soldering resistance in contact with Al-Si-Cu alloy", *Materials proceedings*, 2020, **2**, 1, 28.
5. Vladimir Terek, Aleksandar Miletić, Lazar Kovačević, Dragan Kukuruzović, Branko Škorić, Peter Panjan, Pal Terek, "Surface topography and grain morphology of nanolayer TiAlN/TiSIN coating governed by substrate material and rotation during deposition", *Materials proceedings*, 2020, **2**, 1, 32.
6. Paweł Czarniak, Karol Szymanowski, Beata Kucharska, Agnieszka Krawczynska, Jerzy Robert Sobiecki, Jerzy Kubacki, Peter Panjan, "Modification of tools for wood based materials machining with TiAlN/a-CN coating", *Materials science & engineering. B, Solid-state materials for advanced technology*, 2020, **257**, 114540.
7. Djordje Cica, Halil Çalişkan, Peter Panjan, Davorin Kramar, "Multi-objective optimization of hard milling using taguchi based grey relational analysis", *Tehnički vjesnik*, 2020, **27**, 2, 513-519.
8. Nastja Mahne, Matjaž Panjan, "Obstreljevanje trdnih snovi z ioni. I., Teoretični opis razprševanja", *Vakuumist*, 2020, **40**, 1/2, 10- 21.

Review Article

1. Peter Panjan, Aljaž Drnovšek, Peter Gselman, Miha Čekada, Matjaž Panjan, "Review of growth defects in thin films prepared by PVD techniques", *Coatings*, 2020, **10**, 5, 447.

Published Conference Contribution

1. Pal Terek, Dragan Kukuruzović, Lazar Kovačević, Aleksandar Miletić, Vladimir Terek, Branko Škorić, Peter Panjan, Miha Čekada, "Surface topography and grain morphology of nanolayer TiAlN/TiSIN coating governed by substrate material and rotation during deposition", In: *2nd Coatings and Interfaces Web Conference, 25-31 May, 2020*, Proceedings, sciforum, 2020.
2. Pal Terek, Dragan Kukuruzović, Lazar Kovačević, Aleksandar Miletić, Vladimir Terek, Branko Škorić, Peter Panjan, Miha Čekada, "The influence of CrAlN coating chemical composition on Soldering resistance in contact with Al-Si-Cu Alloy", In: *2nd Coatings and Interfaces Web Conference, 25-31 May, 2020*, Proceedings, sciforum, 2020.
3. Miha Čekada, Peter Panjan, Aljaž Drnovšek, Matjaž Panjan, Peter Gselman, "Growth defects in PVD hard coatings", In: *ICTF-17, 7th International Conference on Thin Films, November 13, 2017, New Delhi, India*, Proceedings, Recent advances in thin films; (Materials Horizons: From Nature to Nanomaterials), Springer, 2020, 35-73.

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.

Head:
Prof. Miran Mozetič

The scientific activities of our research team are in line with the priorities of the Slovenian Strategy of Smart Specialization (S4), which represents the roadmap for the transition to a modern society according to the European Smart Specialisation Strategy (S3). An important task within S4 is the introduction of plasma technologies in agriculture praxis. The plasma techniques have already been approved for specific segments of the food chain, from farm to fork, but the science is still in its infancy. The shortage of appropriate literature encouraged us to prepare a comprehensive monography [1]. The book comprises almost 200 pages and introduces the basic science of non-equilibrium gaseous plasma when interacting with agricultural products. The authors then focus on the influence of plasma processing on an autochthonic Slovenian variety of garlic. The plasma treatment stimulates the germination and growth of these plants, and ultimately better crops. There is a limited range of useful parameters indicating the complex behaviour of the organic matter upon exposure to gaseous plasma. The best treatment conditions are recommended and explained by the effects of neutral plasma radicals, charged particles and radiation in the ultraviolet and vacuum ultraviolet range of wavelengths. The cover page of the monography is shown in Figure 1.

Plasma techniques for virus inactivation were critically evaluated [2]

While the treatment of agricultural products provides an efficient solution for better crops, the plants can suffer from inadequate water quality used for irrigation. Water scarcity remains a global problem, and contamination of the water with microbes that infect plants is a major concern, especially in modern vegetable-production methods such as hydroponics and aeroponics. The plasma treatment of contaminated water represents a powerful microbe-inactivation technique, but an obstacle is the limited applicability at atmospheric pressure. Namely, the plasma radicals' lifetime is limited by the three-body recombination in the gas phase, whose frequency increases with the square of the pressure. Gaseous bubbles in liquid water always assume the ambient pressure, typically slightly above 1 bar. The introduction of hydrodynamic cavitation overcomes this natural obstacle. The liquid water passes a narrow orifice, and the hydrodynamic effect causes the formation of a bubble of water vapour with a pressure close to the water-vapour saturation pressure, which is about 0.03 bar at room temperature. The lifetime of the plasma radicals is thus about 1000-times longer than at atmospheric pressure. This effect was found to be beneficial for sustaining a glow discharge in the bubble inside liquid water. The discharge enabled the formation of stable plasma with a high concentration of radicals and a significant radiation in the virucidal range. Both effects caused the rapid inactivation of the viruses in water. The research group was awarded the first prize for innovation with the highest commercial potential by international judges at the 13th International Technology Transfer Conference. Figure 2 shows the innovators with a prototype of the innovative device.

The virucidal efficiency of gaseous plasma is a hot topic of interdisciplinary research. Many research groups worldwide have tackled this challenge and reported promising results. Different groups used plasma sustained by various discharges and configurations, so the results are difficult to compare. Our research team prepared a review paper to summarise the results and enlighten a few aspects of plasma-virus interaction. The interdisciplinary group of plasma scientists and virologists explained the interaction between the combination of plasma radicals and radiation and viruses. The exact inactivation mechanisms depend on the properties of plasma and virus peculiarities. However, the key mechanisms involved are the irreversible oxidation of virus receptors by plasma radicals of high oxidation potential and bond cleavage in genetic material due to the absorption of plasma radiation. The review paper [2] represents guidance for future scientific work on virus-inactivation mechanisms upon treatment with

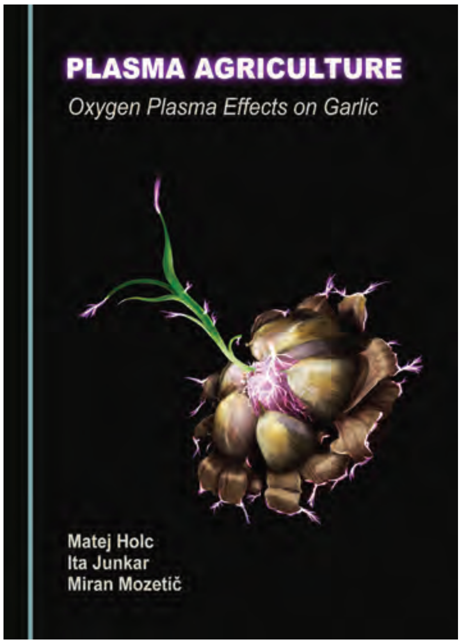

Figure 1: The cover page of our monography on plasma agriculture.

gaseous plasma. This scientific niche is expected to burst in the next future due to the limitations of currently available virucidal methods and the pandemic with SARS-CoV-2. An illustration of the plasma effects on viruses is shown in Figure 3.

Another prospective field of plasma technologies is in medicine. Standard materials commonly employed in body implants do not provide a desired biological response, mainly because they lack the appropriate surface properties. The interaction of proteins and biological cells with the surface is crucial for the long life-span of all implantable devices. Depending on the implant function and position in the body, the surface has to be appropriately conditioned to provide the desired biological response. In the case of vascular implants, the proliferation of endothelial cells is desired. These cells otherwise represent the uppermost layer on the inner side of our natural blood vessels. Furthermore, the adhesion and aggregation of blood platelets should be prevented, as these effects can cause thrombosis. Moreover, in the case of vascular stents, the prevention of the uncontrolled proliferation of smooth muscle cells should be considered, as this could cause restenosis. When blood vessels are badly damaged, they have to be replaced with synthetic ones, often made from knitted polymer (Dacron). The haemo-compatibility of such vascular grafts is inadequate, so various groups worldwide have probed methods for suppressing reactions between the blood constituents and polymeric vascular grafts. An optimal solution would be a heparin coating on the grafts. For decades, heparin has been known as the best anti-coagulant, but the covalent bonding of this substance on the polymer surface has remained a technological challenge. We managed to overcome this by grafting amino groups onto the polymer matrix. The afterglow of ammonia plasma was a source of -NH_2 radicals. Within a limited range of processing parameters, the radicals formed a sub-monolayer film of amino groups, which enabled the covalent grafting of about a monolayer of heparin. Such a surface finish prevented the activation of blood platelets on vascular grafts and thus assured optimal haemocompatibility. The procedure is disclosed in a recently granted EU patent [3].

Figure 2: The interdisciplinary research group gained an award for an innovative technique for water disinfection.

Technology for optimal surface finish of vascular grafts was approved [3]

When blood vessels are not so severely damaged, the vascular stent can be employed to restore the blood flow through an affected vessel. Mostly metallic materials like nitinol, stainless steel, titanium and cobalt-chromium are used for vascular stents. Although these materials provide the desired mechanical stability, their surface features are still far from optimal. Various types of coatings have to be used to prevent thrombosis and restenosis. Our group developed a novel approach based on the surface modification of a NiTi alloy using highly reactive hydrogen and oxygen species. Using this approach, the surface of the NiTi alloy is altered so that a rather thick nanostructured titanium oxide layer is formed on the surface. This layer significantly reduces the adhesion and aggregation of platelets on the surface and reduces surface-induced thrombosis. Our recent studies also showed that the release of toxic Ni ions from the NiTi alloy in the biological environment was reduced. Moreover, the proliferation of endothelial cells was improved, while the proliferation of smooth muscle cells on the surface was reduced. A European patent entitled "Method for treatment medical devices made from nickel-titanium (NiTi) alloys" has been filed. The invention was presented at an international virtual meeting, and we were awarded the "Innovation of the Year" award at the entrepreneurship fair. A picture from the announcement of the winners is in Figure 4.

Our research team is renowned worldwide for its expertise in surface and applied surface sciences. Our expertise provides the characterisation of various materials and the interpretation of the observed surface composition and structure. These activities are often performed in collaboration with other research groups in Slovenia and abroad. The results are usually published in prominent journals. Recently, we have provided expertise in the surface chemistry of Pt catalysts on nanotubular titanium oxynitride-supports [4], fluorinated polymer materials [5], nano-carbon polymer composites [6] and nitrogen-doped graphene-like materials [7].

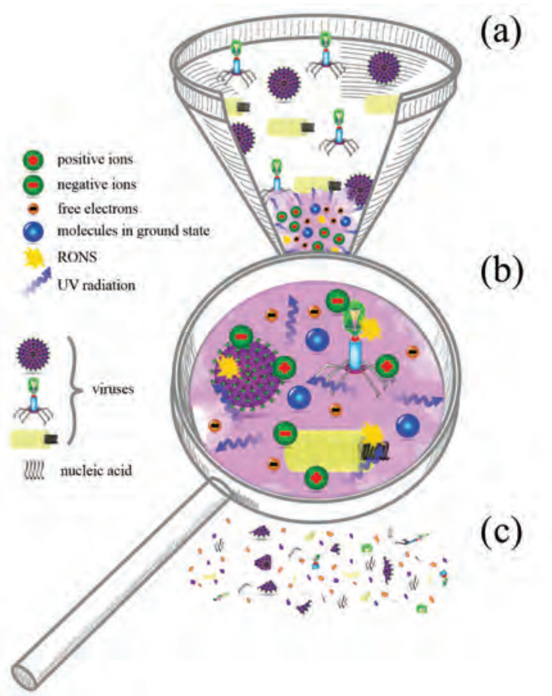

Figure 3: Illustration of plasma-virus interaction. Reprinted from [2].

The research team is among the most innovative groups in Slovenia. In 2020 alone, researchers filed eight patent applications protecting intellectual property rights in different niches of plasma technologies. A team member, Prof. Alenka Vesel, won a medal for the most innovative Slovenian researcher. The medal was granted by the International Intellectual Property Organization (WIPO), based in Geneva, Switzerland. This organisation was founded by the United Nations in 1967. Its mission is to develop and continuously upgrade a balanced and effective system for the protection of intellectual property globally. An international jury consisting of Jeff Skinner, London School of Business (UK), Jon Wulff Petersen, Plougmann Vingtoft (Denmark) and Alojz Barlič, Slovenian Intellectual Property Office, awarded the medal for outstanding results. Alenka Vesel has co-authored seven patents granted by offices that provide a full examination of the innovativeness of a patented solution in the past 10 years. Furthermore, she is also a co-founder of our spin-off company Plasmadis d.o.o., which markets innovative products and services.

Figure 4: Announcement of the "Innovation of the Year" at the 2020 regional fair of innovation and entrepreneurship.

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[5] Lojen, Dane, Zaplotnik, Rok, Primc, Gregor, Mozetič, Miran, Vesel, Alenka. Effect of VUV radiation and reactive hydrogen atoms on depletion of fluorine from polytetrafluoroethylene surface. Applied Surface Science, 533, p. 147356-1-8 (2020).

[6] Oseli, Alen, Vesel, Alenka, Mozetič, Miran, Žagar, Ema, Huskić, Miroslav, Slemenik Perše, Lidija. Nano-mesh superstructure in single-walled carbon nanotube/polyethylene nanocomposites, and its impact on rheological, thermal and mechanical properties. Composites A - Applied science and manufacturing, 136, p. 1-10 (2020).

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Awards and Appointments

1. Asst. Prof. Dr Ita Junkar, Dr Metka Benčina, Prof. Dr Janez Kovač, Prof. Dr Miran Mozetič, Asst. Prof. Dr Rok Zaplotnik: Innovation of the Year, virtual, Regional Virtual Fair on Innovation and Entrepreneurship “Sarajevo 2020”, “Method for treatment medical devices made from nickel-titanium (NiTi) alloys”.
2. Asst. Prof. Dr Ita Junkar: Excellent in Science 2020 Achievement (Odlični v znanosti 2020), Ljubljana, Scientific Council of Slovenian Research Agency (ARRS), “Method of treatment of tools used for isolation of microvesicles, nanovesicles and exosomes”.
3. Asst. Prof. Dr Gregor Primc, Prof. Dr Miran Mozetič, Asst. Prof. Dr Rok Zaplotnik (Jožef Stefan Institute), in collaboration with David Dobnik, Matevž Dular, Arijana Filipić, Ion Gutierrez-Aguirre and Martin Petkovšek: Prize for the Best Innovation with Commercial Potential in 2020, Ljubljana, 13th International Technology Transfer Conference for the innovation, “A scalable method for eco-benign destruction of waterborne microorganisms”.
4. Pia Starič, Asst. Prof. Dr Ita Junkar, Prof. Dr Miran Mozetič, Prof. Dr Katarina Vogel-Mikuš: Best Paper Award, virtual, Sciforum, The 1st International Conference on “Green” Polymer Materials 2020, “Bio-Polymers in the World of Plasma: Effects of Cold Plasma on Seed Surface”.
5. Prof. Dr Alenka Vesel: WIPO medal for inventors, Ljubljana, Slovenian Intellectual Property Office and the World Intellectual Property Organization.


Figure 5: Prof. Alenka Vesel was awarded a WIPO medal

Patents granted

1. Gregor Primc, Miran Mozetič, Rok Zaplotnik, Alenka Vesel, Maja Ravnikar, Jana Žel, Nataša Mehle, Ion Gutiérrez-Aguirre, Arijana Filipić, David Dobnik, Procedure for inactivating virus in water, SI25811 (A), Urad RS za intelektualno lastnino, 30. 09. 2020.
2. Joško Valentinčič, Izidor Sabotin, Matic Resnik, Pavel Drešar, Nejc Matjaž, Marko Jerman, Andrej Lebar, Matej Pleterski, Apparatus and method for cutting an electrically conductive tube, EP3603866 (B1), European Patent Office, 30. 12. 2020.
3. Metod Kolar, Miran Mozetič, Ita Junkar, Alenka Vesel, Martina Modic, Karin Stana-Kleinschek, Method for immobilization of heparin on a polymeric material, EP2997984 (B1), European Patent Office, 03. 06. 2020.
4. Alenka Vesel, Miran Mozetič, Rok Zaplotnik, Gregor Primc, Nina Recek, Procedure for increasing the hydrophilicity of a polymer containing fluorine, SI25862 (A), Urad RS za intelektualno lastnino, 31. 12. 2020.

INTERNATIONAL PROJECTS

1. Small Services
   Prof. Janez Kovač
2. COST CA19110; Plasma Applications for Smart and Sustainable Agriculture
   Asst. Prof. Gregor Primc
   Cost Association Aisbl
3. H2020 - EUROfusion; Education-ED-FU
   Prof. Miran Mozetič
   European Commission
4. H2020 - EUROfusion; WPPFC-PEX-FU, WPPFC-PEX-FU, EUROfusion
   Asst. Prof. Rok Zaplotnik
   European Commission
5. Catalytic Probes for Characterization of Hydrogen Plasma
   Asst. Prof. Gregor Primc
   Slovenian Research Agency
6. Control of Chemical Composition of Thin Films by High Resolution Mass Spectrometry of Secondary Ions
   Prof. Janez Kovač
   Slovenian Research Agency
7. Advanced Catalysts based on Multilayered Vertically Oriented Graphene Nanostructures
   Prof. Alenka Vesel
   Slovenian Research Agency
8. Characterization of Oxygen Plasma Sustained with Powerful Gaseous Discharges
   Prof. Miran Mozetič
   Slovenian Research Agency
9. Low Temperature Plasma Diagnostics and its Applications for Seed Treatment
   Prof. Miran Mozetič
   Slovenian Research Agency
10. Functionalization of Ti-Based Surfaces Using Energy Beams and Plasma for Biomedical Applications
    Asst. Prof. Gregor Primc
    Slovenian Research Agency

RESEARCH PROGRAMMES

1. Thin film structures and plasma surface engineering
   Prof. Miran Mozetič
2. 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. Advanced surface finishing technologies for antibacterial properties of patient specific 3D printed implantable materials
   Asst. Prof. Ita Junkar
5. Hybrid and Reengineered Nanocatalysts for New Purification Routes
   Prof. Janez Kovač
6. Self-organization of plasma in magnetron sputtering discharges
   Prof. Miran Mozetič
7. New startegies for fabrication of biomimetic vascular implants
   Asst. Prof. Ita Junkar
8. Development of new, environment-friendly approaches for plant and human virus inactivation in waters
   Asst. Prof. Gregor Primc
9. Innovative sensors for real-time monitoring of deposition rates in plasma-enhnced chemical vapour deposition (PECVD) systems
   Asst. Prof. Rok Zaplotnik
10. Nanoparticle-reinforced new metal matrix composites manufactured by selective laser melting for tooling industry
    Prof. Miran Mozetič
11. Evaluation of the range of plasma parameters suitable for nanostructuring of polymers on industrial scale
    Prof. Miran Mozetič
12. Selective plasma oxidation of FeCrAl alloys for extended-lifetime of glow plugs for diesel engines
    Prof. Janez Kovač
13. Innovative configuration of inductively coupled gaseous plasma sources for up-scaling to industrial-size reactors
    Prof. Miran Mozetič
14. Carbon nanowalls for future supercapacitors
    Prof. Alenka Vesel
15. Selected area functionalization of polymeric components by gaseous plasma
    Prof. Miran Mozetič
16. Innovative method for purification of wastewater
    Asst. Prof. Gregor Primc
17. Use of gaseous plasma for higher yields and lower use of antifungal agents in agriculture
    Asst. Prof. Ita Junkar
18. Food for future - F4F
    Prof. Alenka Vesel
    Ministry of Education, Science and Sport
19. Potential of biomass for development of advanced materials and bio-based products
    Asst. Prof. Ita Junkar
    Ministry of Education, Science and Sport
20. Innovative ECO plasma seed treatment (for sowing and for human and animal diet/nutrition
    Dr. Nina Recek
    Ministry of Education, Science and Sport
21. Building blocks, tools and systems for the Factories of the Future – GOSTOP
    Prof. Miran Mozetič
    Ministry of Education, Science and Sport
22. Development of nanostructured biosensors for diagnosis/treatment of cancer and surfaces with antibacterial
    Dr. Metka Benčina
    Ministry of Education, Science and Sport
23. Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF)
    Prof. Miran Mozetič
    Ministry of Economic Development and Technology
24. Method for preparation of bacteriostatic surfaces on 3D printed medical implants
    Dr. Matic Resnik
    Ministry of Education, Science and Sport
25. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
    Prof. Miran Mozetič
    Slovenian Research Agency
26. 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
27. Income from Coowners of Invention for Reimbursement of Costs for IP Protection in the Case of EVT140_Mozetič_Carbon Nanowall
Prof. Miran Mozetič
Nagoya University

NEW CONTRACTS

1. L-project co-financing: Innovative method for purification of wastewater
Asst. Prof. Gregor Primc
Induktio d. o. o.
2. L-project co-financing: Selected area functionalization of polymeric components by gaseous plasma
Prof. Miran Mozetič
Elvez, d. o. o.

VISITOR FROM ABROAD

1. Prof. Dr Petr Špatenka, Czech Technical University in Prague, Prague, the Czech Republic, 25 February 2020

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5. Asst. Prof. Gregor Primc
6. Prof. Alenka Vesel
7. Asst. Prof. Rok Zaplotnik

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10. Dean Popović, B. Sc.
11. Dr. Nina Recek
12. Dr. Matic Resnik

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14. Dane Lojen, B. Sc.
15. Domen Paul, B. Sc.
16. Pia Starič, B. Sc.
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21. Janez Trtnik

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Original Article

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DEPARTMENT OF SOLID STATE PHYSICS F-5

Our research programme focuses on the study of the structure and dynamics of disordered and partially ordered condensed matter at the atomic and molecular levels, with special emphasis on phase transitions. The purpose of these investigations is to discover the basic laws of physics governing the behaviour of these systems, which represent the link between perfectly ordered crystals, on the one hand, and amorphous matter, soft condensed matter and living systems on the other. Such knowledge provides the key to our understanding of the macroscopic properties of these systems and is an important condition for the discovery and development of new, multifunctional materials, nanomaterials and biomaterials for new applications. An important part of the research program is devoted to the development of new experimental methods and techniques in the field of magnetic resonance 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 Jožef Stefan Institute is performed in close collaboration with Department of Physics at the Faculty of Mathematics and Physics of the University of Ljubljana, Institute of Mathematics, Physics and Mechanics and the Jožef Stefan International Postgraduate School. In 2020, the research was performed within three research programs:

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

I. Research Programme "Magnetic Resonance and Dielectric Spectroscopy of New Smart Materials"

The research of the programme group *Magnetic Resonance and Dielectric Spectroscopy of New Smart Materials* in 2020 was focused on physical phenomena in condensed matter at the atomic and molecular levels. The purpose of the investigations was to discover the basic laws of physics governing the behaviour of the investigated systems. The attained knowledge provides 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 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 of ultra-cold atoms.

The research group has observed asperomagnetism in high-entropy alloys, determined the quantum critical point in Ce_3Al, investigated the surface quantum properties of topological insulators via the detection of Dirac electrons, developed thick piezoelectric HfO_2-based films, investigated the relation between dielectric and electrocaloric response in relaxor ferroelectrics, observed soliton waves in matter by the method of ultra-cold atoms and contributed importantly to the understanding of quantum and topological magnetism.

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

In 2020 the members of the programme group published 65 original scientific papers in international peer-reviewed scientific journals and one book chapter. Among these, one paper was published in Nature Physics (IF = 19.2), one in Nature Communications (IF = 12.1), one in Angewandte Chemie, Intl. Ed. (IF = 12.9), one in Physical Review Letters (IF = 8.4) and one in Advanced Materials (IF = 27.4).

The investigations were focused on the following research fields:

1. Speromagnetism and asperomagnetism in the Tb-Dy-Ho-Er-Tm high-entropy alloy

In the paper "Speromagnetism and asperomagnetism as the ground states of the Tb-Dy-Ho-Er-Tm IDEAL high-entropy alloy" by M. Krnel, *et al*., Intermetallics **117**, 106680 (2020), we addressed the nature of the collective magnetic state in an ideal high-entropy alloy (HEA) based on rare-earth (RE) elements, representing a magnetically concentrated system with all the lattice sites occupied by localized magnetic moments and containing randomness and frustration due to chemical disorder. Being a "metallic glass on a topologically ordered lattice", HEAs possess simultaneously the properties of an ordered crystal and an amorphous glass. The influence of this crystal-glass duality on the collective magnetic state was studied experimentally on a hexagonal Tb-Dy-Ho-Er-Tm (TDHET) HEA, composed of RE elements with zero pair mixing enthalpies that ensure completely random mixing of the elements and very similar atomic radii that minimize lattice distortions, representing a prototype of an ideal HEA. The TDHET HEA is characterized by probability distributions of the atomic moments $P(\mu)$, the exchange interactions $P(J)$, the magnetocrystalline anisotropy $P(D)$, and the dipolar interactions $P(H_d)$. Based on measurements of the static and dynamic magnetizations, the magnetization $M(H)$ curves (Fig. 1), the thermo-remanent magnetization, the specific heat and the magnetoresistance, we found that the collective magnetic state of the TDHET is temperature dependent, forming a speromagnetic (SPM) state in the temperature range between about 140 and 30 K and an asperomagnetic (ASPM) state below 20 K. In the intermediate temperature range between 30 and 20 K, a spin glass (SG) state is formed, representing a transition state between the speromagnetic and asperomagnetic states. The observed temperature evolution of the magnetic ground state in the TDHET HEA upon cooling in the sequence SPM→SG→ASPM is a result of temperature-dependent, competing magnetic interactions. The distribution of the exchange interactions P(J) shifts continuously on the J axis from the high-temperature SPM-type with the average interaction biased towards a net negative value, $\bar{J}<0$, through the SG-type with $\bar{J}=0$, to the low-temperature ASPM-type with $\bar{J}>0$. This shift is a band-structure effect, closely linked with the crystallinity of the spin system, which the TDHET HEA shares with the topologically ordered crystals. The probability distributions $P(\mu)$, $P(J)$, $P(D)$, and $P(H_d)$ are, on the other hand, a consequence of the chemical disorder, a property that the TDHET HEA shares with amorphous magnets. Both features, the topologically ordered lattice and the amorphous-type chemical disorder, essentially determine the magnetic state of an ideal, RE-based HEA.

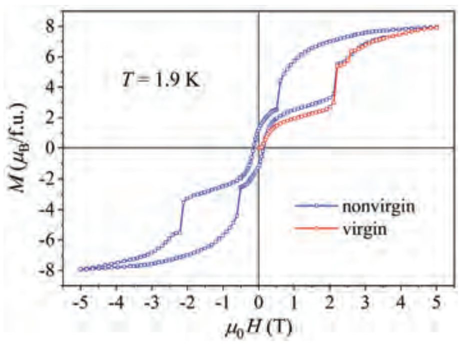

Figure 1: Complicated magnetization versus the magnetic field curve of the TDHET HEA, revealing the interplay of the speromagnetic and asperomagnetic spin ordering.

2. Anisotropic quantum critical point in Ce_3Al

In the paper "Anisotropic quantum critical point in the Ce_3Al system with a large magnetic anisotropy" by S. Vrtnik, *et al*., J. Phys. Commun. 4, 105016 (2020), we studied experimentally the magnetic field driven quantum critical point (QCP) in the Ce_3Al magnetically anisotropic intermetallic compound, which shows both antiferromagnetic (AFM) ordering and heavy-fermion behaviour. Measurements of the magnetic susceptibility, the magnetoresistance and the specific heat on a Ce_3Al monocrystalline sample performed down to 0.35 K in magnetic fields up to 9 T demonstrate that the QCP is anisotropic regarding the orientation of the magnetic field relative to the magnetically easy direction (Fig. 2). An external magnetic field drives the AFM transition continuously towards zero temperature when applied in the (*a*,*b*) easy plane, reaching the QCP at the critical field $B_c^{a,b} = 4.6 \pm 0.4$ T, where a quantum phase transition from the AFM to the paramagnetic state takes place. The magnetoresistance experiments below 1 K indicate that intermediate magnetic states might have formed near the QCP. For the field applied along the *c* hard direction, the QCP has not been observed within our experimental range of the magnetic field. The anisotropic, magnetic field driven QCP in the Ce_3Al results from competition of the exchange interaction with the Zeeman interaction in the presence of a large magnetocrystalline anisotropy. The anisotropy of the QCP is a consequence of the fact that the magnetic anisotropy locks the magnetization into the easy plane and cannot be pulled out of the plane by the field available in the laboratory. Consequently, only the component of the magnetic field vector that lies in the easy plane participates in the QCP formation. In AFM systems with a large magnetic anisotropy, the magnetic field driven QCP is a continuous variable of the magnetic field's vector orientation relative to the easy direction.

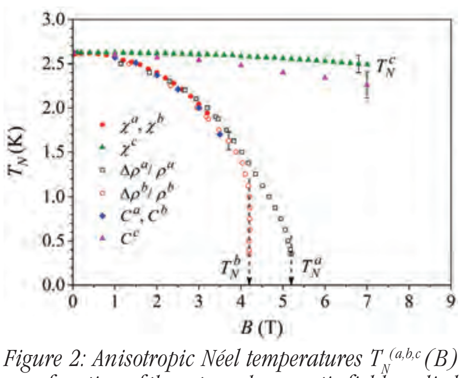

Figure 2: Anisotropic Néel temperatures $T_N^{(a,b,c)}(B)$ as a function of the external magnetic field applied along different crystallographic directions. The Néel temperatures were determined from the magnetic susceptibility, the magnetoresistance and the specific heat (the method is indicated in the legend).

3. Surface quantum properties of topological insulators via the NMR-detection of Dirac electrons

In the paper "Resolving Dirac electrons with broadband high-resolution NMR" by W. Papawassiliou, J. Dolinšek, *et al*., Nat. Commun. **11**, 1285 (2020), we investigated the surface quantum properties (SQPs) of a topological insulator (TI) Bi_2Te_3 in a nanoplatelet morphology. Detecting the metallic Dirac electronic states on the surface of TIs is critical for a study of important SQPs, such as Majorana zero modes, where simultaneous probing of the bulk and edge electron states is required. However, there is a particular shortage of experimental methods, showing at an atomic resolution how Dirac electrons extend and interact with the bulk interior of nanoscale TI systems. By applying advanced broadband solid-state ^{125}Te nuclear magnetic resonance (NMR) methods on Bi_2Te_3 nanoplatelets, we succeeded in uncovering the hitherto invisible NMR signals with magnetic shielding that is influenced by the Dirac electrons, and we subsequently showed how the Dirac electrons spread inside the nanoplatelets (Fig. 3). In this way, the spin and orbital magnetic susceptibilities induced by the bulk and edge electron states were simultaneously measured with an atomic scale resolution, providing a pertinent experimental approach in the study of SQPs.

4. **Stabilization of the perovskite phase in epitaxial thin films via increased interface roughness**

Perovskite $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT) exhibits excellent piezo- and dielectric properties; however, only in the absence of the pyrochlore phase, which results from the PbO loss during synthesis. Pulsed-laser deposition was used to prepare PMN-PT thin films on $LaNiO_3/SrTiO_3$ (LNO/STO) substrates. We found that the bottom electrode has an immense influence on the properties of the overgrown active layer. Specifically, the use of LNO as the electrode material, strongly stabilizes the perovskite phase and significantly expands the process window for the preparation of phase-pure PMN-PT, as compared to a direct deposition on STO substrates. By understanding the mechanism (the stabilization is achieved primarily due to the increased interface roughness, which offers more Pb-binding sites), we were able to prepare a STO/Nb:STO template with a rough surface, which strongly enhanced the stability of the perovskite phase and, consequently, improved the electrical properties of films. The developed approach can be used to design templates for various device configurations. The work was published in U. Gabor, D. Vengust, Z. Samardžija, A. Matavž, V. Bobnar, D. Suvorov, M. Spreitzer, Stabilization of the perovskite phase in PMN-PT epitaxial thin films via increased interface roughness, Applied Surface Science **513**, 145787 (2020).

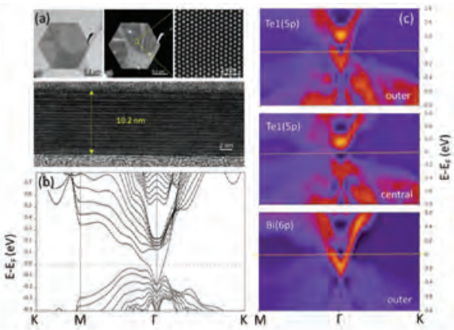

Figure 3: Band-structure analysis and Dirac states of stoichiometric Bi_2Te_3 nanoplatelets. (a) High-resolution TEM and HAADF image of Bi_2Te_3 nanoplatelets (top view and cross-section). (b Band structure of a 9-quintuplets-thick (~10 nm) Bi2Te3 slab. (c) The projected k-resolved DOS of the Te(1) |5p⟩ and Bi |6p⟩ orbital states at the outer (edge) quintuplets, and the Te(1) |5p⟩ orbital states at the central quintuplet. Dirac states are only observed at the edge quintuplets.

5. **Development of thick piezoelectric HfO_2-based films**

In HfO_2-based films, which are mainly prepared by atomic-layer deposition, the desired ferroelectric properties typically vanish for thicknesses above 50 nm. In collaboration with researchers from the Luxembourg Institute of Science and Technology, we have successfully fabricated 1-μm-thick piezoelectric La:HfO_2 films using chemical solution deposition. After identifying the optimal La content, the film thickness was increased from 45 nm to 1 μm. Polarization and strain measurements evidence the persistence of the ferroelectric properties and even a slight improvement due to a better orientation of the polar axis at higher thicknesses. The fine-grained microstructure is believed to help in stabilizing the polar orthorhombic $Pca2_1$ phase in developed films, paving the way towards cost-efficient HfO_2-based sensor and actuator applications. The work was published in T. Schenk, N. Godard, A. Mahjoub, S. Girod, A. Matavž, V. Bobnar, E. Defay, S. Glinšek, Toward thick piezoelectric HfO_2-based films, Physica Status Solidi – Rapid Research Letters **14**, 1900626 (2020).

6. **Relationship between dielectric and electrocaloric responses in relaxor ferroelectrics**

The correlation between dielectric permittivity and electrocaloric (EC) temperature change (ΔT_{EC}) was investigated in $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ relaxor ferroelectric ceramics. Such a relation would help to predict the temperature range wherein the EC effect is the highest. We showed that the peak of the dielectric permittivity is always at a higher temperature (T_m) than the peak of ΔT_{EC}, and that the temperature gap between both maxima progressively increases with increasing applied DC bias. The results, which are explained in terms of the electric field-temperature phase diagram of relaxor systems, thus reveal that T_m can only roughly mark the upper boundary of the temperature-electric-field window, where the EC responsivity is the highest. The work was published in L. Fulanović, A. Bradeško, N. Novak, B. Malič, V. Bobnar, Relation between dielectric permittivity and electrocaloric effect under high electric fields in the $Pb(Mg_{1/3}Nb_{2/3})O_3$-based ceramics, Journal of Applied Physics **127**, 184102 (2020).

7. **Study of nanostructured materials' ordering and caloric effects in electronic ceramics and soft materials**

We have shown, by direct measurements and simulations, the existence of the large elastocaloric effect in main-chain liquid-crystal elastomers that can be tuned by the crosslinkers' density. We continued with the studies of the ferroelectric properties, the electromechanical and electrocaloric effect in novel bulk lead-free materials. We demonstrated that these materials could,

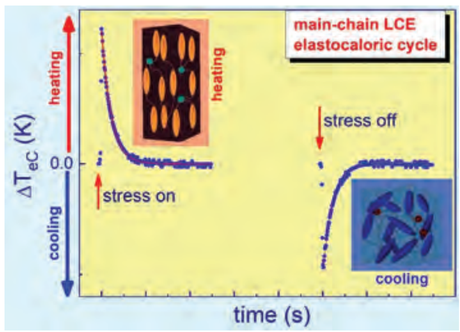

Figure 4: Elastocaloric cooling cycle in main-chain liquid-crystal elastomers.

in all properties, replace materials based on lead. Besides, we have shown that graphene nanoparticles decorated by CoPt could stabilize for optical applications interesting blue phases in liquid crystals. The above results have been published in 17 articles in international scientific journals. Recent papers of our group on multiferroics, multicalorics and soft materials have been cited more than 400 times in 2020. The work was published in five articles.

8. Rapid determination of NQR frequencies using field-cycling magnetic resonance

The main advantage of measuring the nuclear quadrupole resonance (NQR) frequencies is the possibility to study the electron charge distribution in the vicinity of the observed atomic nucleus, for example, the chemical bonds formed by the atom. Due to its high resolution, NQR can also be used as an analytical technique, which clearly distinguishes between molecules and crystal polymorphs. NQR can also be used to study the microscopic state of order in the sample as, for example, in case of an exchange or reorientation. We describe a modified Slusher-Hahn's nuclear quadrupole double resonance (NQDR) technique, which can be used for the rapid location of NQR frequencies. The technique is based on the adiabatic magnetic field cycling between a high magnetic field B_0 and zero magnetic field, where we replace the phase-modulated RF magnetic field by a series of frequency sweeps that pass the NQR frequency (Fig. 5). The new technique enables a rapid scan of the NQR spectrum independent on the NQR frequency. The work was published in T. Apih, A. Gregorovič, V. Žagar, J. Seliger, A rapid determination of nuclear quadrupole resonance frequencies using field-cycling magnetic resonance and frequency modulated RF excitations, J. Magn. Reson. **310** (2020) 106635.

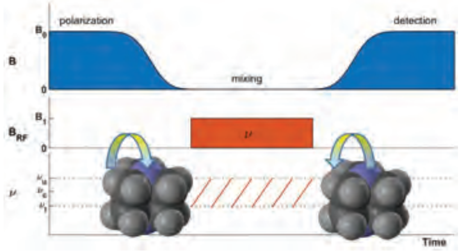

Figure 5: Adiabatic magnetic field cycling between a high magnetic field B_0 and zero magnetic field, where we replace the phase-modulated RF magnetic field by a series of frequency sweeps that pass the NQR frequency.

9. TiO_2 nanostructures doped with Eu^{3+} and Nd^{3+} for temperature sensing

Lanthanide-based optical nanothermometers, operating in the physiological temperature range between 15 °C and 50 °C, with excitation and emission in the first biological transparent window are of special interest for biological applications. In this context, trivalent europium-doped titanium oxide (Eu^{3+}:TiO_2) nanoparticles were prepared via a sol-gel method and their spectroscopic properties were studied. We observed that the intensities of the excitation bands for the $^7F_0 \rightarrow {}^5D_0$ (576 nm) and $^7F_2 \rightarrow {}^5D_0$ (610 nm) transitions, monitoring the $^5D_0 \rightarrow {}^7F_4$ (700 nm) transition have a strong dependence on the temperature (Fig. 6). This dependence, which is explained in terms of the thermal coupling between the Eu^{3+}:^7F_J levels, was used for the construction of an optical nanothermometer. The work was published in L.J. Borrero-González, Selene Acosta, Carla Bittencourt, Maja Garvas, Polona Umek, L.A.O. Nunes. Eu^{3+}-doped titanium oxide nanoparticles for optical thermometry in the first biological window. *Optical Materials* **101** (2020) 109770.

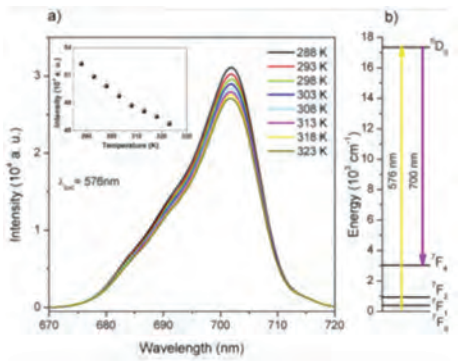

Figure 6: a) Photoluminescence temperature dependence for the emission of the $^5D_0 \rightarrow {}^7F_4$ transition with excitation $^7F_0 \rightarrow {}^5D_0$. The inset shows the integrated intensity of the emission band. (b) Simplified energy-level diagram of Eu^{3+} ion illustrating the excitation and radiative transitions.

10. Transformation of $H_2Ti_3O_7$ nanotubes to anatase nanoparticles

The purpose of the transformation study of $H_2Ti_3O_7$ nanotubes into anatase nanoparticles was to prepare TiO_2 nanoparticles of different morphologies for subsequent toxicity studies. The transformation reactions of the $H_2Ti_3O_7$ nanotubes were conducted under various hydrothermal conditions, as well as with calcination in air. In the case of transformations under hydrothermal conditions, it was found that besides T and pH, the presence of a capping agent in the reaction mixture had an effect on the shape and size of the formed TiO_2 nanoparticles (Fig. 7). TiO_2 nanoparticles of various shapes were later used in toxicity studies. The work was published in Kokot, Hana, Kokot, Boštjan, Sebastijanović, Aleksandar, Podlipec, Rok, Krišelj, Ana, Čotar, Petra, Pušnik, Mojca, Umek, Polona, Pajk, Stane, Urbančič, Iztok, Koklič, Tilen, Štrancar, Janez, et al. Prediction of chronic inflammation for inhaled particles: the impact of material cycling and quarantining in the lung epithelium. *Advanced materials* **32** (2020) 2003913.

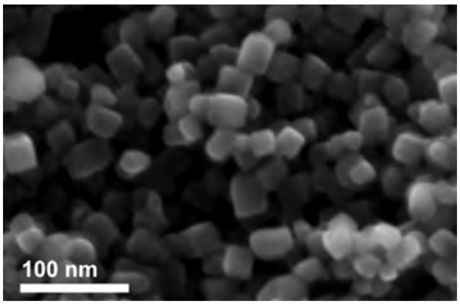

Figure 7: Conversion of $H_2Ti_3O_7$ nanotubes under hydrothermal conditions in an alkaline medium yield anatase nanoparticles of cuboid morphology.

11. Investigation of orientational order parameter in polymer-dispersed liquid-crystal elastomers

Andraž Rešetič and Boštjan Zalar with coworkers and partners from Italy and the Czech Republic investigated the orientational order parameter in polymer-dispersed liquid-crystal elastomers (PDLCE). Their thermomechanical properties are governed by the degree of imprinted particle alignment, achieved during the synthesis in a strong magnetic field. Deuterium NMR was used on the samples with various degrees of imprinted liquid-crystal elastomer (LCE) particle alignment (Fig. 8). The recorded spectra were simulated using the discrete reorientational exchange model. It was determined that the maximum order of the LCE particle alignment is achieved in magnetic fields larger than 5 T, when the dispersion of the orientational distribution settles a 20° and the orientational order parameter at a value of 0.54. The thermomechanical behavior of the same samples follow the above patern. The work was published in Andraž Rešetič, Jerneja Milavec, Valentina Domenici, Blaž Zupančič, Alexej Bubnov, Boštjan Zalar, Deuteron NMR investigation on orientational order parameter in polymer dispersed liquid crystal elastomers, **Phys. Chem. Chem. Phys. 22** (2020) 23064.

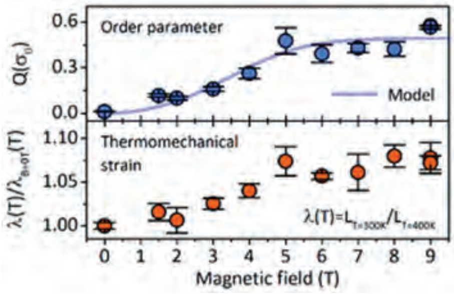

Figure 8: Experimentally determined orientational order parameter $Q(\sigma_0)$ (upper graph) and thermomechanical response (lower graph) of the same PDLCE samples. The maximum order parameter is acieved for $B \geq 5$ T at the value of $Qmax(\sigma_0) = 0.54$. Thermomechanical responses were determined on several pieces of the same sample by measuring the length change when heated from 300 K to 400 K.

12. Quantum and topological magnetism

Martin Klanjšek, in collaboration with partners from France, tested the previously proposed analytical expression for the NMR spin-lattice relaxation rate due to the enhancement of critical spin fluctuations in quasi-one-dimensional spin systems in the vicinity of the magnetic ordering transition. The expression is experimentally confirmed by excellent fits to the published temperature dependence of the spin-lattice relaxation rate data in two representative quasi-one-dimensional spin compounds, $(C_7H_{10}N)_2CuBr_4$ (DIMPY) and $BaCo_2V_2O_8$. A positive test also provides a direct and convenient experimental determination of the Tomonaga-Luttinger-liquid interaction parameter, which is found in very nice agreement with the theoretical predictions. The work was published in the paper M. Horvatić *et al.*, "Direct determination of the Tomonaga-Luttinger parameter *K* in quasi-onedimensional spin systems", *Phys. Rev. B* **101**, 220406(R) (2020).

Matej Pregelj, Andrej Zorko, Denis Arčon and Martin Klanjšek, in collaboration with partners from France, Switzerland and Austria, investigated a frustrated spin-1/2 chain β-$TeVO_4$ by nuclear magnetic resonance (NMR) at high magnetic fields. They were looking for the theoretically predicted spin-nematic phase, i.e., an intriguing state of matter that exhibits higher multipolar order but lacks the usual long-range dipolar order. The research team found that the detected missing fraction of the magnetization, probed by NMR frequency shift, is thermally activated and is thus not a fingerprint of the spin-nematic behaviour, as previously proposed. This fact undermines the presence of the spin-nematic phase in the investigated compound. Moreover, it highlights the importance of careful considerations of a temperature-dependent NMR shift that has been overlooked in previous studies of spin nematicity. The work was published in the paper M. Pregelj *et al.*, "Thermal effects versus spin nematicity in a frustrated spin-1/2 chain", *Phys. Rev. B* **102**, 081104(R) (2020).

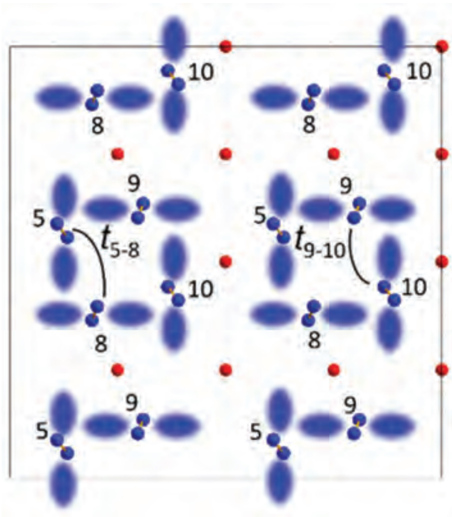

Figure 9: Orbital ordering in Rb_4O_6 drives the quantum magnetic state of weakly coupled spin dimers.

Matej Pregelj, Andrej Zorko and Denis Arčon, in collaboration with partners from Croatia, France and Switzerland, used torque magnetometry to study a frustrated spin-1/2 chain β-$TeVO_4$. They investigated the anisotropy of spin-density-wave (SDW), vector-chiral and spin-stripe phases in magnetic fields of up to 5 T. Their results show that the magnetic-field-induced spin reorientation occurs in the SDW and in the spin-stripe phases in fields greater than 2 Tesla. The presented results should help establish the model of anisotropic magnetic interactions, which are responsible for the formation of complex magnetic phases in β-$TeVO_4$ and similar low-dimensional quantum spin systems. The work was published in the paper M. Herak *et al.*, "Magnetic-field-induced reorientation in the spin-density-wave and the spin-stripe phases of the frustrated spin-1/2 chain compound β-$TeVO_4$", *Phys. Rev. B* **102**, 024422 (2020).

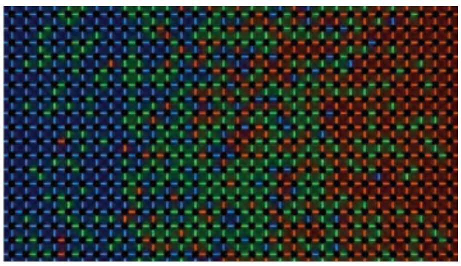

Figure 10: Simulation of random exchange bonds on a 2D square spin lattice.

In an extensive study, Tilen Knaflič, Peter Jeglič, Andrej Zorko and Denis Arčon, together with colleagues from Germany, investigated low-temperature quantum magnetism in Rb_4O_6. This study was a continuation of the previous one on the related Cs_4O_6, where we discovered charge ordering similar to the famous Verwey transition. In this study, we discovered a second structural instability at lower temperatures, which is probably related to the orbital ordering (Fig. 9). The low-temperature instability defines the magnetic properties, as experiments with electron paramagnetic resonance at high fields unambiguously show quantum magnetism of weakly coupled spin dimers. The research has been published as "Editor's suggestion" in the article T. Knaflič et al., "Spin-dimer ground state driven by consecutive charge and orbital ordering transitions in the anionic mixed-valence compound Rb_4O_6", *Phys. Rev. B* **101**, 024419 (2020).

Matjaž Gomilšek, in collaboration with partners from the United Kingdom, explored the influence of randomized exchange bonds on the magnetism of a $S = 1/2$ quantum Heisenberg antiferromagnet (QHAF) on a quasi-2D square lattice (Fig. 10). The researchers found that magnetic order is strongly suppressed by quenched exchange strength randomness (realized by chemical substitution in $(QuinH)_2Cu(Cl_xBr_{1-x})_4{\cdot}2H_2O$, where QuinH = Quinolinium = $C_9H_8N^+$ and $0 \leq x \leq 1$), with an extended quantum-disordered phase forming over a wide range of intermediate substitution levels, where no ground-state magnetic order is observed. They propose a simple and general energetics-based model of competing local magnetic orders in disordered magnets, and find that it describes the observed critical

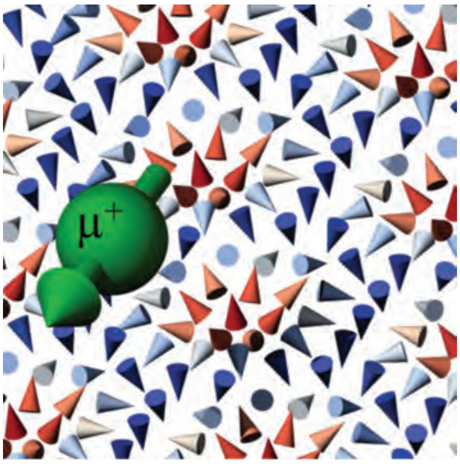

Figure 11: Sketch of a muon over a lattice of topologically non-trivial magnetic Néel skyrmions.

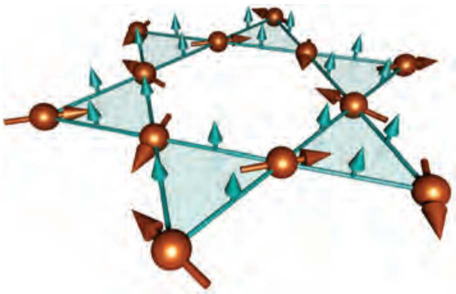

Figure 12: Magnetic ordering on the kagome lattice resulting from Dzyaloshinskii-Moriya interaction.

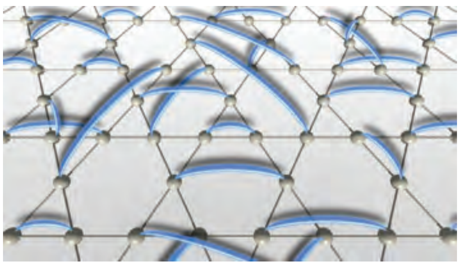

Figure 13: Formation of valence bonds in the spin-liquid ground state of the quantum kagome lattice.

substitution levels in the studied compound. Due to the ubiquity of quenched disorder in many of the most interesting QHAF and other frustrated magnetic materials, this study should have wide implications in the field of quantum magnetism. The work was published in the paper F. Xiao *et al.*, "Magnetic order and disorder in a quasi-two-dimensional quantum Heisenberg antiferromagnet with randomized exchange", *Phys. Rev. B* **102**, 174429 (2020).

Matjaž Gomilšek, in collaboration with partners from the United Kingdom, explored the influence of low levels of chemical substitution on the magnetism of $GaV_4S_{8-y}Se_y$. The researchers showed that the materials in this series exhibit lattices of Néel skyrmions (exotic topological spin textures) over a range of elevated temperatures by studying their dynamics via muon spin relaxation (μSR), as shown in Figure 11. They also found that chemical substitution stabilizes additional skyrmionic precursor states that persist down to even lower temperatures. Finally, at the lowest temperatures, the researchers discover a gradual crossover from cycloidal magnetic order to a ferromagnetic ground state in both the $y = 0$ and the $y = 0.1$ materials, and reveal that chemical substitution leads to an inhomogeneous local spin density in this series of materials. The discovered rich phase diagram and non-trivial substitutional effects make $GaV_4S_{8-y}Se_y$ an especially interesting series of topological magnets. The work was published in the paper T. J. Hicken *et al.*, "Magnetism and Néel skyrmion dynamics in $GaV_4S_{8-y}Se_y$", *Phys. Rev. Research* **2**, 032001(R) (2020).

Tina Arh, Matjaž Gomilšek, Matej Pregelj, Martin Klanjšek and Andrej Zorko studied, with collaborators from the UK, USA and China, the effect of perturbations on the ground state of the quantum kagome spin lattice. They found that magnetic ordering in the investigated compound $YCu_3(OH)_6Cl_3$ is triggered by a sizable Dzyaloshinskii-Moriya interaction that enhances spin correlations within the kagome planes (Fig. 12). They confirmed experimentally the theoretically predicted role of this interaction and the corresponding phase diagram. The findings were published in the article T. Arh *et al*., "Origin of Magnetic Ordering in a Structurally Perfect Quantum Kagome Antiferromagnet", *Phys. Rev. Lett.* **125**, 027203 (2020).

Andrej Zorko and collaborators from France and India determined the exact nature of the spin-liquid ground state in herbertsmithite, an archetypal representative of the quantum kagome spin lattice. The question of the existence of a spin gap in this compound has remained unanswered for many years, despite numerous experimental studies. With an in-depth nuclear magnetic resonance experiment, the researchers proved that the ground state is gapless, and thus showed good agreement with recent theoretical predictions that envisage a Dirac spin-liquid as the ground state of the kagome lattice (Fig. 13). The work was published in the article P. Khuntia *et al*., "Gapless ground state in the archetypal quantum kagome antiferromagnet $ZnCu_3(OH)_6Cl_2$", *Nat. Phys.* **16**, 469 (2020).

13. Superconductivity

Denis Arčon, Peter Jeglič, Martin Klanjšek and Nejc Janša studied superconductivity emerging from the paradigmatic quantum spin liquid in TaS_2, together with colleagues from the F7 and F1 departments. In the study, they focused on the 1T-TaS_2 layered system, which was systematically doped with Se. Using Ta-181 NQR and Se-77 NMR they demonstrated that after the parent spin liquid is destroyed and replaced by the metallic state, antiferromagnetic correlations remain and define the metallic state. Such correlations might be important for the emerging superconducting state in the strong coupling limit. The work has been published in the article I. Benedičič et al., "Superconductivity emerging upon Se doping of the quantum spin liquid 1T-TaS_2", *Phys. Rev. B* **102**, 054401 (2020).

Žiga Gosar, Nejc Janša, Tina Arh, Peter Jeglič, Martin Klanjšek and Denis Arčon, together with colleagues from the University of Texas at Dallas, investigated superconductivity of quasi-one-dimensional metal $Rb_2Mo_3As_3$. Spin-lattice relaxation rate showed a characteristic power-law temperature dependence, which is a signature of Tomonaga-Luttinger liquid (TLL) but in the surprising regime of attractive interactions. The additional presence of three-dimensional electronic band stabilizes superconductivity at the surprisingly high critical temperature. In the article published in Ž. Gosar et al., "Superconductivity in the regime of attractive interactions in the Tomonaga-Luttinger liquid", *Phys. Rev. B* **101**, 220508(R) (2020) we also discussed the relevance of TLL physics for the emerging superconductivity.

14. Functional materials

Denis Arčon participated in a study of the Li_2VO_2F cathode material. Using pulsed and continuous electron paramagnetic resonance (EPR), he showed that the sample, which was charged at the potential 4.1 V, shows EPR spectrum that is a sum of V^{4+} ($3d^1$) and superoxide O_2^- signals. In particular, the discovery of the later component is important as its presence probably influences the reversibility of charging cycles. The research has been published in J. H. Chang et al., "Superoxide formation in Li_2VO_2F cathode material – a combined computational and experimental investigation of anionic redox activity", *J. Mater. Chem. A* 8,16551 (2020).

Tilen Knaflič and Denis Arčon participated in the international collaboration to study potassium-intercalated Tetracene solid. The study is a part of ongoing collaboration in the field of interacalatic aromatic solids. We used EPR method to show that K_2Tetracen is a nonmagnetic insulator. The study has been published in C. I. Hiley et al., "Crystal Structure and Stoichiometric Composition of Potassium-Intercalated Tetracene" *Inorg. Chem*. 59, 12545–12551 (2020).

Peter Jeglič, Tadej Mežnaršič and Denis Arčon, in collaboration with partners from Japan, reported the first study of rubidium-loaded LSX zeolite employing complementary macroscopic and microscopic probes. The ^{87}Rb NMR spin-lattice relaxation of the rubidium cluster component showed temperature-independent behavior. This confirmed the metallic ground state, despite the fact that rubidium clusters are formally confined in the insulating framework. The work was published in the paper P. Jeglič *et al.*, "Metallic State in Rubidium-Loaded Low-Silica X Zeolite", *J. Phys. Soc. Jpn.* 89, 073706 (2020).

Andrej Zorko and other collaborators from the JSI and Norway studied the influence of cobalt doping and the annealing atmosphere on the electrical conductivity and the electrical polarization switching in $BiFeO_3$ ceramics. They proposed a mechanism of hardening, which assumes the existence of two types of pinning centers. The results of the study will help in further optimizing local and macroscopic conductivity, as well as hardening properties of these technologically important ceramics. The results were published in the article M. Makarovič *et al*., "Tailoring the electrical conductivity and hardening in $BiFeO_3$ ceramics", *J. Eur. Ceram. Soc.* 40, 5483 (2020).

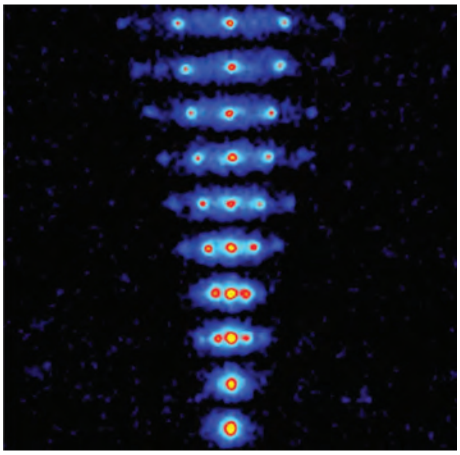

Figure 14: Pairs of matter-wave jets emitted from a modulated cesium Bose-Einstein condensate.

15. Cold atoms

Tadej Mežnaršič, Tina Arh, Erik Zupanič and Peter Jeglič demonstrated the emission of correlated atom jets from a driven matter-wave soliton in a quasi-one-dimensional optical trap (Fig. 14). All the stages of the Bose jet emission were captured in a simple model based on the 1D Gross-Pitaevskii equation, giving an insight into the dynamics of density waves that precede the emission. In the limit of vanishing high-order jets beyond-mean-field number correlations of jet pairs were observed. The results were published in T. Mežnaršič *et al*., "Emission of correlated jets from a driven matter-wave soliton in a quasi-one-dimensional geometry", *Phys. Rev. A* 101, 031601(R) (2020).

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

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

Using theoretical and numerical approaches, we explain the flow of light through complex structures of topological solitons in frustrated chiral nematics. In a thin layer of unwound cholesteric, we show the chirality amplified periodic self-focusing of a strong laser beam and the formation of similariton. By modelling, we show that with topological defects in an ion-doped nematic liquid crystal we can manipulate charge distributions on chemically homogeneous surfaces. For material flows and morphological dynamics of topological defect lines and loops in 3D active nematics, theoretical and numerical approaches show the importance of the local orientation order surrounding the defects.

Light control by topological solitons in chiral nematics

Topological solitons appearing in different areas of physics are fascinating, localized perturbations of ordering fields enjoying topological protection. We demonstrate refraction, reflection, and lensing of weak laser beams by various topological solitons in frustrated chiral nematic liquid crystals. We show how the interactions of light with such topological solitons are well described using a generalized Snell's law and ray-tracing models. These might lead to new means for controlling the flow of light for use in optics and photonics. The study was made by group members from the Jožef Stefan Institute and the Faculty of Mathematics & Physics at University of Ljubljana in collaboration with the group of Ivan Smalyukh

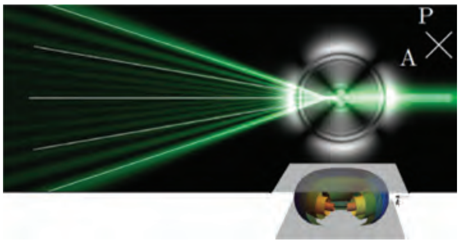

Figure 15: Simulated green light beam lensing from a toron in the unwounded cholesteric layer. Intensity of green colour corresponds to the intensity of light. White lines are obtained by simple ray tracing. The 100-μm toron with the director field illustrated in the inset is visualized with a white-light polarization image.

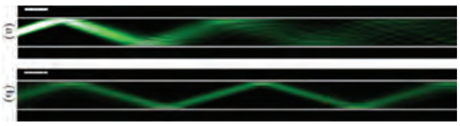

Figure 16: Propagation of a tilted Gaussian light beam inside the unwounded cholesteric layer in the linear (a) and nonlinear – similariton (b) optical regime. The white bars represent 10 μm.

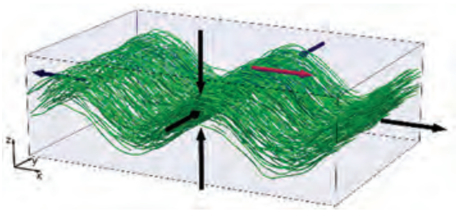

Figure 17: Nematically aligned bundles of microtubules (green) first condense vertically into a ribbon that subsequently forms wrinkles due to active extensile stress.

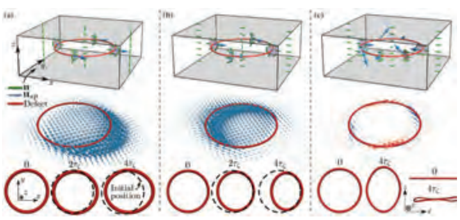

Figure 18: Flows and dynamics of different active nematic defect loops with zero topological charge

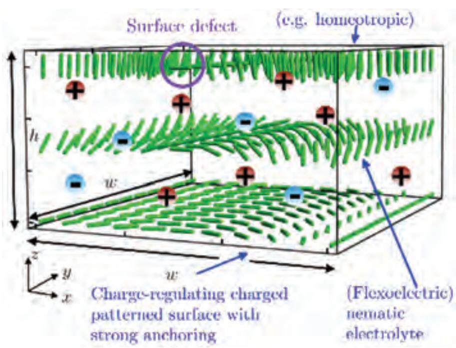

Figure 19: Surface-induced electric-charge variability caused by nematic defects.

from University of Colorado in Boulder. The paper (*Physical Review X, 2020, DOI:* 10.1103/PhysRevX.10.031042*)* was highlighted in *APS Physics Focus* by the editorial article "Liquid-Crystal Vortices Focus Light".

Chirality-enhanced periodic self-focusing of light in frustrated chiral nematics

In achiral liquid crystals, the reorientation of molecules around laser beams with appropriate power is responsible for the generation of spatial optical solitons called "nematicons". We present numerical, experimental, and theoretical evidence of a strong link between chirality and the nonlinear optical response of frustrated chiral liquid-crystal systems. In unwounded chiral nematics, the frustration caused by a confinement incompatible with their lowest-energy states allows a relatively weak light to locally destabilize the initially uniform orientational fields and thus boost their nonlinear optical responses. This yields self-focusing and the formation of similaritons. In short, our study opens, at a fundamental level, a new research paradigm of chirality-enhanced nonlinear optical effects, thus suggesting a range of self-focusing-based applications such as low power light self-actuated flat lenses or all-optical information processing based on spatial optical solitons interacting with chiral topological solitons. The study was made in a collaboration by the Jožef Stefan Institute and the Faculty of Mathematics & Physics at University of Ljubljana with the group of Ivan Smalyukh from University of Colorado in Boulder (*Physical Review Letters, 2020, DOI:* 10.1103/PhysRevLett.125.077801*)*.

Wrinkling instability in 3D active nematics

In this experimental and theoretical study we focus on a 3D active nematic consisting of microtubules, kinesin motors, and a depleting agent. It shows rich dynamics evolving from a nematically ordered space-filling distribution of microtubule bundles towards a flattened and contracted 2D ribbon that undergoes a wrinkling instability and subsequently transitions into a 3D active turbulent state. The interplay between the depletion forces and the kinesin motors thus leads to both a contractile stress that compresses the ribbon and an extensile stress that leads to the wrinkling instability. On the macroscopic scale, we used a continuum theory to explain the instability and predict the wavelength of the wrinkles that form. We supplemented the results with a detailed simulation at the molecular scale (using the Cytosim package) that reproduced the dynamics based on the properties of single kinesin motors. We found that the produced forces nearly cancel out, but a small asymmetry in the distribution leads to the build-up of the extensile stress. Whereas the wrinkle wavelength strongly correlates with their formation time, as predicted by the continuum theory, it is independent of the ATP concentration. The 3D to quasi-2D and back to 3D transition in our system represents a novel path of self-organization in active soft matter. The study was mostly performed at Max Planck Institute for Dynamics and Self-Organization in Göttingen *(Nano Letters, 2020, DOI:*10.1021/acs.nanolett.0c01546).

Three-Dimensional Active Defect Loops

We describe the flows and morphological dynamics of topological defect lines and loops in three-dimensional active nematics and show, using theory and numerical modelling, that they are governed by the local profile of the orientational order surrounding the defects. Analysing a continuous span of defect loop profiles, ranging from radial and tangential twist to wedge profiles, we show that the distinct geometries can drive the material flow perpendicular or along the local defect loop segment, whose variation around a closed loop can lead to net loop motion, elongation, or compression of shape, or buckling of the loops. We demonstrate a correlation between the local curvature and the local orientational profile of the defect loop, indicating dynamic coupling between the geometry and the topology. To address the general formation of defect loops in three dimensions, we show their creation via bend instability from different initial elastic distortions. The work was performed in a collaboration between the University of Warwick (Prof. G. Alexander), the Faculty of Mathematics and Physics at the University of Ljubljana and Department of Condensed Matter Physics at the Jožef Stefan Institute *(Physical Review Letters, 2020, DOI:* 10.1103/PhysRevLett.124.088001*)*.

Topological-Defect-Induced Surface Charge Heterogeneities in Nematic Electrolytes

We show that the topological defects in an ion-doped nematic liquid crystal can be used to manipulate the surface-charge distribution on chemically homogeneous, charge-regulating external surfaces, using a minimal theoretical model. In particular, the location and type of the defect encodes the precise distribution of surface charges, and the effect is enhanced when the liquid crystal is flexoelectric. We demonstrate the principle for patterned surfaces and charged colloidal spheres. More generally, our results indicate an interesting approach to control the surface charges on external surfaces without changing the surface chemistry *(Physical Review Letters, 2020, DOI:* 10.1103/PhysRevLett.125.037801*)*.

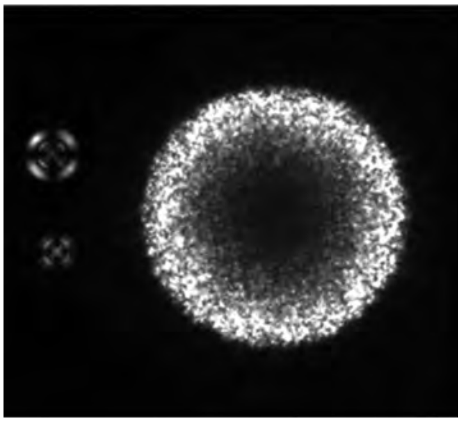

Figure 20: Thermal quenching of liquid crystal with 5-ns exposure time.

Speckle-free liquid-crystal microscopy with nanosecond illumination

We present a setup for speckle-free, low-light microscopy imaging using 5-ns exposure times. The design is based on the stroboscopic principle and uses fast and incoherent fluorescent emission from a solution of a fluorescent dye, excited by a picosecond laser pulse. The proposed solution of Rhodamine in ethanol put in a glass cuvette gives an excellent image quality with high contrast, excellent stability and tuneable coherence. The setup was used for the photographic measurements with 5-ns exposure time, demonstrated in the imaging of a thermally quenched 5CB liquid crystal, which enables studies of the Kibble-Zurek mechanism of topological defect nucleation and growth at sub-microsecond time resolution and extremely fast cooling rates of ~40,000 K/s. The research was conducted in collaboration with the Faculty of Mathematics and Physics and the Faculty of Pharmacy at University of Ljubljana. (*Liquid Crystals, DOI:* 10.1080/02678292.2020.1790049).

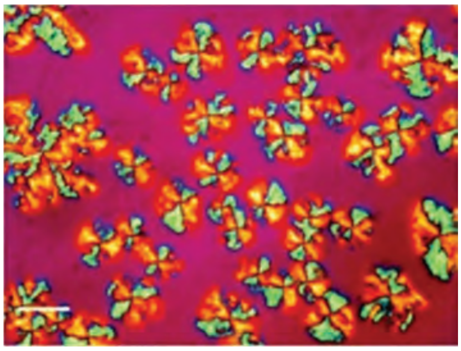

Figure 21: Bright flower-like domains in the inverse nematic gel.

Bright flower-like domains in inverse nematic gels

We discovered that mixing the gelator 12-HSA with a nematic liquid crystal results in the creation of localised flower-like domains with a higher concentration of the gelator than the surrounding medium. The gelator in these domains forms fibres, which interact with the molecules of the liquid crystal and stabilise its director into a spiral, toron-like structure. We examined their structure by optical and confocal microscopy. The nematic liquid crystal in the volume around the domains is achiral, but all the domains exhibit the same handedness. The research was conducted in collaboration with the Faculty of Mathematics and Physics at University of Ljubljana and the Raman Institute in Bangalore. *(Soft matter, 2020, DOI:* 10.1039/C9SM02547B*)*.

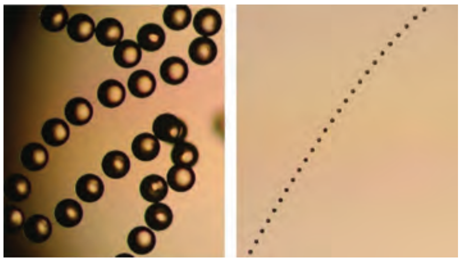

Figure 22: Two necklaces made of LC droplets connected by a micro-tether.

Nematic liquid-crystal necklace structure made by a microfluidic system

We succeeded in fabricating necklace structures made of liquid-crystal droplets that are tens of micrometres in diameter and are connected by birefringent micro-tethers made of a PVA liquid-crystal composite. Micro-tethers can be elastically stretched by applying external force and the elastic constant of the tether was determined using laser tweezers. The Whispering Gallery Modes circulating inside the individual droplets in the necklace structure were also observed. Research was made in collaboration with AIST in Tsukuba (*Langmuir, DOI:* 10.1021/acs.langmuir.0c00101*)*.

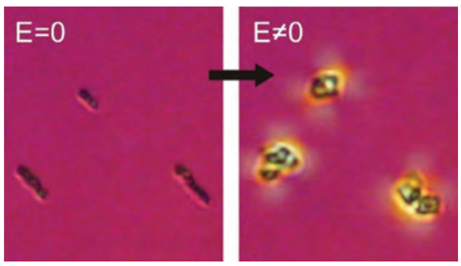

Figure 23: Micro-platelets are rotated in a liquid crystal by the external electric field.

Electric-field-induced reorientation of ferroelectric platelets in a liquid crystal

We demonstrated that ferroelectric micro-platelets can be reoriented in a nematic liquid crystal by linear coupling to an external electric field. The electric dipole moment of the platelets is perpendicular to the plane of platelets and provides torque that rotates the platelets. The experiments were made in dispersions of platelets in a zero dielectric anisotropy nematic liquid crystal, which excludes the reorientation of the dispersion via the dielectric coupling of a liquid crystal. Liquid-crystal molecules are reoriented only via the rotation of platelets. (*Liquid Crystals, DOI:* 10.1080/02678292.2020.1785026)

Graphene derivatives, liquid crystal, and CdS/TiO_2 hybrid matrices: optoelectronic and biotechnological aspects

Different assemblies of nanomaterial and related new switchable device technologies are reviewed. Complex systems consisting of graphene and its derivatives, hydrogen-bonded liquid crystals, and semiconducting nanoparticles or nano wires are addressed. Seamless stable assemblies are enabled by relatively strong hydrogen bonds. Of particular interest are the configurations that can undergo sensitive stimulus-induced electro-optical changes between states exhibiting significantly different effective properties. Such assemblies could be exploited in flexible electronics, high contrast ratio smart displays, optoelectronic devices, sensors (monitoring inflammability, explosive nature, or toxicity of chemicals), bio-sensing, and antimicrobial applications. Cost-effective technologies, enabling

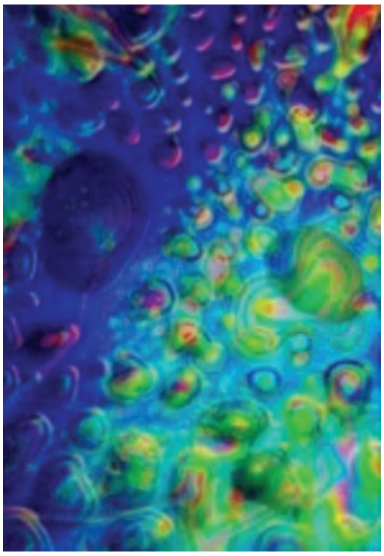

Figure 24: Polarizing-microscopy texture of a hybrid composite.

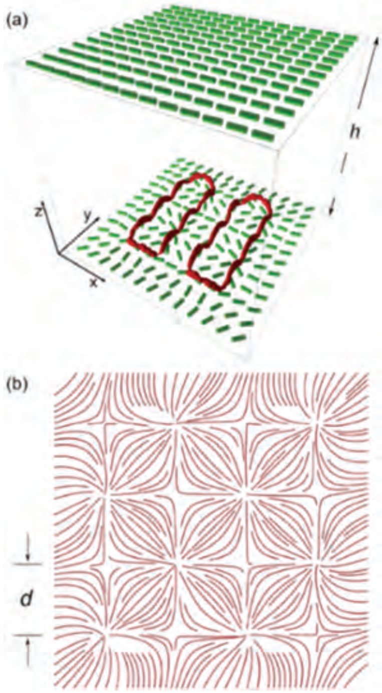

Figure 25: a) Typical defect configuration, b) bottom plate enforced nematic pattern.

large scalability and seamless heterogeneous integration are presented *(Critical Reviews in Solid State and Materials Sciences, 2020, DOI:* 10.1080/10408436.2020.1805295*).*

Reconfigurable multi-stable topological defect patterns

We report on robust theoretical and experimental investigations in which an external electric field is used to switch between pre-determined stable chargeless disclination patterns in a nematic cell. The different defect configurations are stabilized by a master substrate that enforces a lattice of surface defects exhibiting zero total topological charge value. Theoretically, we model disclination configurations using a Landau-de Gennes phenomenological model. Experimentally, we enable diverse defect patterns by implementing an in-house-developed Atomic Force Measurement scribing method, where NLC configurations are monitored via polarised optical microscopy. We show numerically and experimentally that an "alphabet" of up to 18 unique line defect configurations can be stabilized in a 4×4 lattice of alternating s=±1 surface defects, which can be "rewired" multistably using appropriate field manipulation. Our proof-of-concept mechanism may lead to a variety of applications, such as multi-stable optical displays and rewireable nanowires. Research was performed in collaboration with Case Western Reserve University Cleveland *(Physical Review Research, 2020, DOI:* 10.1103/PhysRevResearch.2.013176*).*

Emergent collective colloidal currents generated via exchange dynamics in a broken dimer state

We investigated the dynamics of paramagnetic colloidal particles confined between two planes. When subjected to a precessing magnetic field, they show a rich phase diagram depending on the rotation frequency, cell thickness, precession angle and particle density. We used linear-stability analysis to theoretically predict the boundaries between the phases. They include single particles on a hexagonal lattice, synchronously and asynchronously rotating particle pairs. Between them, a particularly interesting phase emerges where dimers form and break transiently. Therefore, an edge current emerges where particles at one boundary move in one direction and those at the opposite boundary in the opposite direction. These results demonstrate how similar physical phenomena can exist across a range of length scales. The research was conducted in the collaboration of researchers from University of Barcelona Max Planck Institute for Dynamics and Self-Organization in Göttingen *(Science Advances, 2020, DOI:*10.1126/sciadv.aaz2257*).*

Generation of microdroplets and microbeads with nanometre precision

We demonstrated that it is possible to produce small droplets and solid spheres of an unprecedented monodispersity of 1 nm and 20 nm, respectively. For the droplets, the corresponding coefficient of variation is only 0.0042 %, which improves the size precision by three orders of magnitude compared to standard production methods such as reported in microfluidics. Encoding of short words and numbers has been demonstrated by producing three beads with predefined sizes. The stored information has been read from the emitted spectrum. The potential to store information on such a small scale, which can be read purely through the spectrum, has the potential for barcoding various products, for security applications and even for tagging and tracking of individual live cells. The article that was featured on the back cover of the journal *Lab on a Chip* was made in collaboration with the Harvard Medical School *(Lab on a Chip, 2020, DOI:* 10.1039/C9LC01034C*).*

Blood flow limits endothelial cell extrusion in the zebrafish dorsal aorta

We studied the formation of the dorsal aorta, the main artery in the developing zebrafish embryo. We combined confocal imaging on live embryos with a theoretical prediction of the stress distribution in the tissue surrounding the blood vessel. The latter is amplified in the proximity of another blood vessel, but reduced in the proximity of the stiff notochord. We show that cells migrate towards a direction that coincides with the maximum pulsatile stress during the heartbeat. On the other hand, reduced blood flow facilitates cell extrusion, pointing to a mechanism that regulates the blood-vessel diameter. Our study demonstrates how the formation and growth of blood vessels depend on an intricate interplay of chemical signals, tissue mechanics and fluid dynamics. The research was conducted in the collaboration of researchers from Université de Strasbourg and Max Planck Institute for Dynamics and Self-Organization in Göttingen *(Cell Reports, 2020, DOI:*10.1016/j.celrep.2020.03.069).

Control of viscosity in biopharmaceutical protein formulations

Controlling the viscosity of concentrated protein solutions (usually reducing) is an open challenge, with major recent relevance in protein formulations for biopharmaceutical, medical, food, and other applications. It is of major importance to be able to establish control over the combination of viscosity-affecting additives and adequate protein stability, usually at high protein concentrations. Here, we demonstrate the control and manipulation of the viscosity profile of a selected protein solution (monoclonal antibody of immunoglobulin gamma type – IgG) of direct biopharmaceutical relevance, by identifying elementary viscosity contributions via selected additives that target different protein-protein interactions. Specifically, a combined study of viscosity control and protein aggregation is performed with the viscosity characterized by microfluidic measurements and protein aggregation by size-exclusion chromatography, where aggregation data is further supplemented with conformational stability measurements via thermal and chemical protein denaturation. More generally, we show control over the interplay of viscosity, potency and stability in a distinct protein system, as a general contribution to understanding the viscosity in different colloidal, biological, and soft materials. The work was performed as collaboration between the Lek Pharmaceuticals d.d, part of Novartis, the Faculty of Mathematics and Physics and the Biotechnical Faculty at the University of Ljubljana and Department of Condensed Matter Physics at the Jožef Stefan Institute. *(J. Coll. Int. Sci., 2020, DOI:* 10.1016/j.jcis.2020.06.105*)*

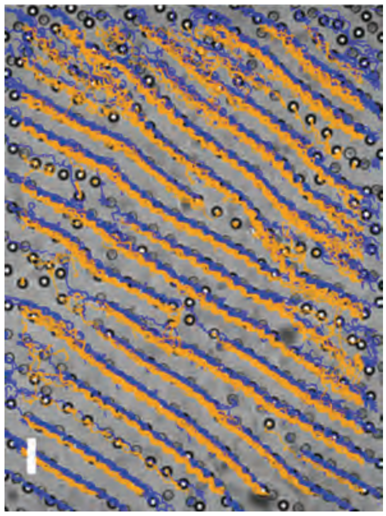

Figure 26: Trajectories of magnetic particles in a precessing field. Particles in the proximity of both planes move in opposite directions (blue and yellow traces).

Antimicrobial coatings based on MoO_3 nanowires

A novel antimicrobial nanocomposite was designed from inert biocompatible PVDF-HFP and water-soluble PVP polymers with incorporated MoO_3 nanowires. Dissolving in water in a concentration of 5mg/ml, it lowers the pH value to 4.6 in 5 min. Anti-microbial activity studied in collaboration with the Biotechnical Faculty University in Ljubljana was explained by a two-step action: in the first stage, MoO_3 dissolves, causing a drop in pH, which then triggers the hydrolysis of the PVP polymer and the release of the ammonium salt. Complete deactivation of *Staphylococcus aureus*, *Listeria monocytogenes*, *Escherichia coli* and *Pseudomonas aueroginosa* was achieved within 6 h, and deactivation of *Penicilium verrucosum* and *Pichia anomala* within 24 h (*Journal of Nanomaterials 2020, DOI:* 10.1155/2020/9754024*).*

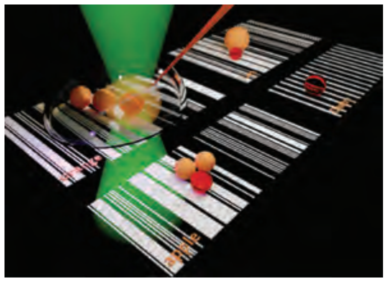

Figure 27: Graphic of four groups of microbeads, each with embedded information, which can be read by a laser.

New quasi-two-dimensional W_nO_{3n-1} crystals

We synthesized new quasi-two-dimensional tungsten oxide crystals, which nucleate by epitaxial growth on the $W_{19}O_{55}$ nanowires. In a single platelet, several stoichiometric phases were identified for the first time: $W_{18}O_{53}$, $W_{17}O_{50}$, $W_{16}O_{47}$, $W_{15}O_{44}$, $W_{14}O_{41}$, and W_9O_{26}. The structure was directly resolved from high-resolution electron microscopy images and modelled using electron and X-ray diffraction data. These layered crystals show a new kind of polycrystallinity, where crystallographic shear planes accommodate an oxygen deficiency and at the same time contribute to the stability of a particular phase. (*Nanoscale, 2020, DOI:* 10.1039/D0NR02014A).

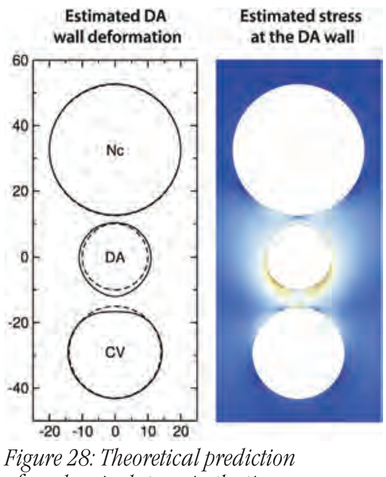

Figure 28: Theoretical prediction of mechanical stress in the tissue surrounding the dorsal aorta (DA).

Spatial ordering of the charge-density waves in $NbSe_3$

The ordering of the two incommensurate charge-density waves (CDWs) in the quasi-one-dimensional $NbSe_3$ structure was studied using low-temperature scanning–tunnelling microscopy (PRB 102, 075442 (2020)). Larger (100) van der Waals surfaces were analysed using one-dimensional Fourier transforms along the trigonal prismatic columns. The procedure enabled unambiguous differentiation between both CDWs, modulating individual columns and allowed quantitative comparison of modulation amplitudes along different columns of the same type. The results suggest the formation of CDW nanodomains. The possibility of interchanging both CDWs along columns forming symmetry-related pairs results in a charge difference, which is supposed to be the possible origin of CDW sliding. The paper was published in collaboration with a researcher from Canada (Physical Review B, 2020, *DOI:* 10.1103/PhysRevB.102.075442*).*

The ultra-high-TP charge-density wave in the monoclinic phase of NbS_3

We reported on high-temperature studies of electrical conductivity of the monoclinic phase of NbS_3 type-II (J. Alloys & Compounds, 854, 157098 (2020)). The compound was shown to be stable up to a temperature $T \approx 550$ K. At $T_{P0} \approx 450–475$ K a step-like growth of conductivity was observed, clear evidence that T_{P0} is the temperature of a third, high-temperature CDW formation. The synchronization at moderate frequencies, 10–50 MHz, demonstrates coherent sliding of CDW-0. The charges condensed in this CDW show a relatively high density and, at the same time, extremely low mobility. Their mobility appears low in the single-particle states as well, giving a plausible clue to the surprising dielectric-like temperature variation of σ above T_{P0}. The paper was published in collaboration with groups from Taiwan and Russia *(Journal of Alloys and Compounds, 2020, DOI:* 10.1016/j.jallcom.2020.157098*).*

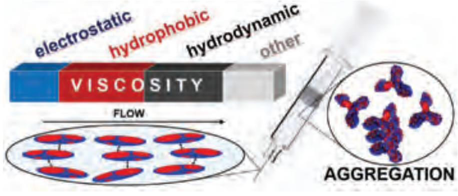

Figure 29: Control of viscosity in biopharmaceutical protein formulations via design of different protein interactions.

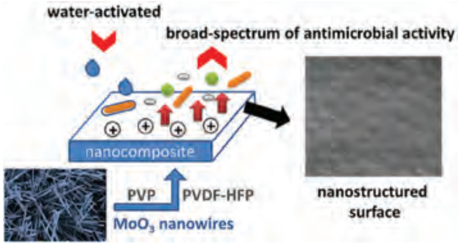

Figure 30: Schematic illustration of antimicrobial activation of PVDF-HFP/PVP/MoO_3 nanowires composite.

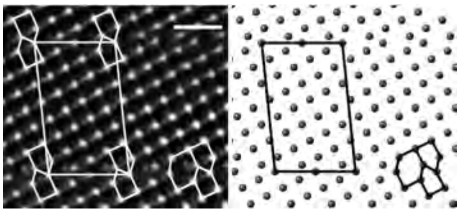

Figure 31: HRTEM image and its simulation of the $W_{16}O_{47}$ phase with pentagonal and hexagonal tunnels at crystallographic shear planes. The scale bar is 1 nm.

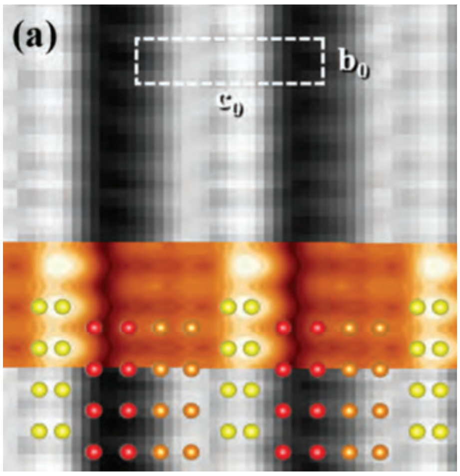

Figure 32: STM image of the surface of NbSe3 shown with the uppermost Se atoms and a DFT simulated STM image.

Spontaneous Antiferromagnetic Ordering in a Single Layer of $(BETS)_2GaCl_4$ Organic Superconductor

The fabrication of well-defined and atomically clean interfaces between materials of different orders are of fundamental interest to engineer novel functionalities and to study emergent phenomena in condensed-matter physics. Our study was focused on the interplay between electronic orders of a hybrid mix of nested antiferromagnetic molecular chains and superconducting molecular stripes at the single-layer limit. The results of low-temperature scanning–tunnelling microscopy and spectroscopy have shown that low-level vibronic and magnetic excitations that dominate the higher temperature phase are absent below T_c, which point to their cooperative existence and possible renormalization to mediate superconductivity in such d-wave superconductors. The paper was published in collaboration with the group at Nihon University, Tokyo (*Advanced Electronic Materials, 2020, DOI:* 10.1002/aelm.202000461).

Air pollution by nanoparticles released during a football match

We measured air pollution with nanoparticles during a derby between the football clubs NK Olimpija Ljubljana and NK Maribor on March 2019 in Stožice. The fan groups of both teams, Green Dragons and Viola Maribor, lit torches and pyrotechnics in support of their clubs, despite the ban. The number of nanoparticles ranging in size from 30 nm to 300 nm in the air when the torches were lit increased by 1200 %, and the players inhaled 300 % more particles than in a low-pollution environment. Chemical analysis showed that in addition to carbon, there were also elements that were potentially toxic and used for colour effects and as fuel: strontium (red), barium (green), potassium, magnesium and chlorine (*Atmospheric Environment 2020, DOI:* 10.1016/j.atmosenv.2020.117567*)*.

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, micro-spectroscopies 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 health care 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 aging population. The investment into the new super-resolution STED system opened a variety of fluorescence microscopy approaches: STED microscopy and two-photon (2PE) microscopy, multichannel spectrally resolved fluorescence lifetime imaging (spFLIM), fluorescence micro-spectroscopy (FMS). These, coupled with optical tweezers, can be used to examine interactions between materials, nanomaterials and cell 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 enables 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 the diffusion in confined geometries with the use of modulated gradients.

Epidemiological evidence suggests that the inhalation of pollutants, including the nanoparticles in polluted air, contributes to around 4 million deaths worldwide. However, it is still not known which nanoparticles are responsible. In collaboration with the National Research Centre for the Working Environment (NRCWE) (Denmark) we have shown that among several different types of anatase TiO_2 nanoparticles only the nanotubes triggered chronic inflammation in mice.

We developed the world's first animal-free in-vitro model for the prediction of chronic inflammation after nanoparticle inhalation, which we published in the prestigious journal Advanced Materials.

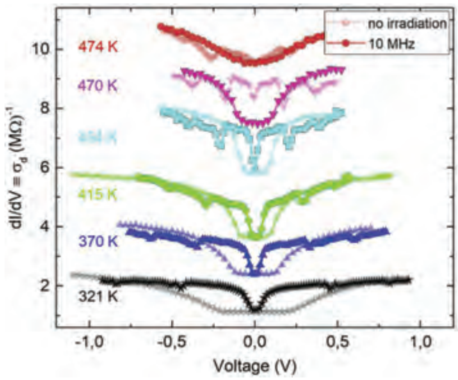

Figure 33: Temperature dependence of I-V curves with and without the RF irradiation applied.

After our discovery in 2019 that epithelial cells passivate some nanomaterials on their surface, reducing the destructive effect of interactions between nanomaterials and various structures in cells (e.g., nucleus, actin networks, inner membranes; all observed by STED microscopy) we have developed the world's first animal-free in-vitro model for the prediction of chronic inflammation after nanoparticle inhalation. It is based on the complex mechanism discovered within intensive collaborative research as a part of a work package that we led within the €8m European Horizon 2020 SmartNanoTox project. The mechanism of nanomaterial toxicity is based on three key events: 1) formation of agglomerates of nanoparticles and biomolecules on the surface of lung epithelial cells, 2) toxicity of the material to macrophages, and 3) cell signalling, all linked in a perpetual cycle of events. The resulting publication in the prestigious journal Advanced Materials was selected as the frontispiece by the editor and is currently in the top 5% of all research outputs scored by Altmetric. This enormous collaborative work has been directed by our researchers T. Koklič and J. Štrancar and co-authored by many of the world's top toxicologists from Germany, France, Denmark, Canada, Finland, Sweden, Ireland, and UK.

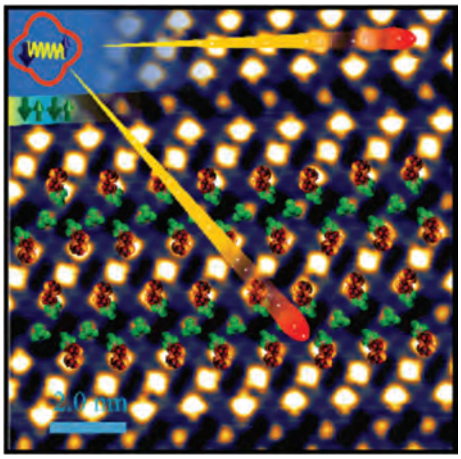

Figure 34: Hybrid order of two ground states where molecular magnetic chains are nested within a single-layer organic superconductor

In collaboration with the University of Oxford (UK), we have been developing advanced fluorescence microscopy and microspectroscopy methods for the characterisation of local molecular environments. We greatly expanded the flexibility of super-resolution fluorescence correlation spectroscopy (STED-FCS) by integrating faster detection electronics. We introduced an aberration-resilient depletion pattern for more reliable STED-FCS measurements in 3D and applied adaptive optics to characterise the diffusion in challenging cellular environments. We also investigated new probes for gentler super-resolution imaging technique RESOLFT. For our future development of advanced nanospectroscopies, we obtained and started a new ARRS research project (J7-2596) in collaboration with the Visual Cognitive Systems Laboratory from the Faculty of Computer and Information Science, University of Ljubljana.

The research work conducted within the ARRS project Microspectroscopy-based optimization of the effects of laser pulses on the retina (L7-7561) were published in two peer-reviewed papers. Here we report the capabilities of the in-house-developed 2-photon laser system (Laboratory for Photonics and Laser Systems (FOLAS), Faculty of Mechanical Engineering as LBF partner) for the retinal tissue theragnostics and the capabilities of fluorescence hyperspectral imaging with a bespoke data-analysis algorithm for tracking blood coagulation and oxygenation dynamics conducted in *ex-vivo* retinal vessels. Besides publications, the extensive work on the projects has resulted in a granted European patent "Image-processing apparatus and image-processing method for detection of irregularities in tissue" (PCT/SI2018/050007, EP2018713384).

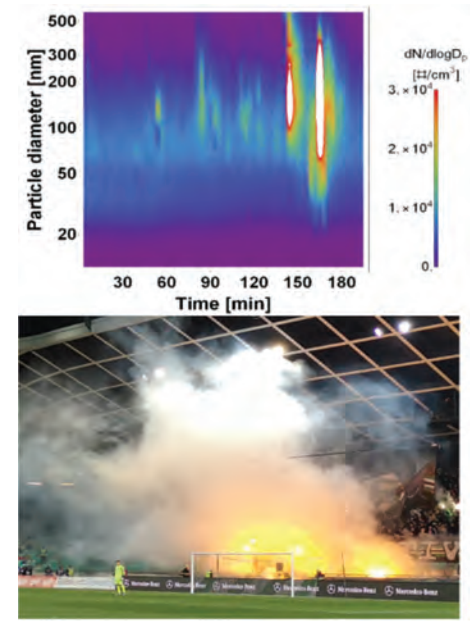

Figure 35: Use of flares and pyrotechnics during a match caused an up to 12-fold increase in the number concentration of nanoparticles in the air.

In the framework of the next ARRS project (L2-9254) focused on the spatial and temporal design of the laser systems for minimally invasive ophthalmological applications, our STED laser system was upgraded with a new beam line for testing a newly developed adaptive laser system (Laboratory for Photonics and Laser Systems (FOLAS), Faculty of Mechanical Engineering as LBF partner). Diagnostics and therapy capabilities together with the new algorithm and concepts for theragnostic approaches were characterized on human retinal tissue. The findings of the research will be published in 2021.

Further studies have been performed for the project focused on nano-temperature mapping done in collaboration with the Laboratory for Heating Technology LTT, Faculty of Mechanical Engineering. Temperature profiling for micro-boiling studies has been tested with a newly developed temperature-sensitive organic and inorganic molecules and particles. Based on the preliminary findings, new collaboration with Advanced Materials Department (K9) was established for the continued experimental work in 2021.

A lot of work has been dedicated to the running project Crossing Borders and Scales (CROSSING) focused on the advanced applications of correlative microscopy (CM) using state-of-the-art high-resolution imaging and analysis techniques provided at the JSI and partnering HZDR. The continued research focused on nanoscale CM characterization of nanomaterial interacting with the biological matter (model lung epithelium, neuron network) contributed to the high-impact-journal publication and to a better understanding of the molecular events potentially responsible for toxicological behaviour. New analytical CM approaches have been tested and planned for 2021 to provide further details of the relevant biological system.

Another activity in 2020, led by the Laboratory of Biophysics, was the submission of the application for the involvement in the JSI Infrastructure program for the period from 2022–2027. Based on vast expertise and the available infrastructure of advanced and multimodal optical microscopies, we have applied, together with the few JSI departments, for the new centre called the Center for advanced optical microscopies, which would be a part of CEMM centre.

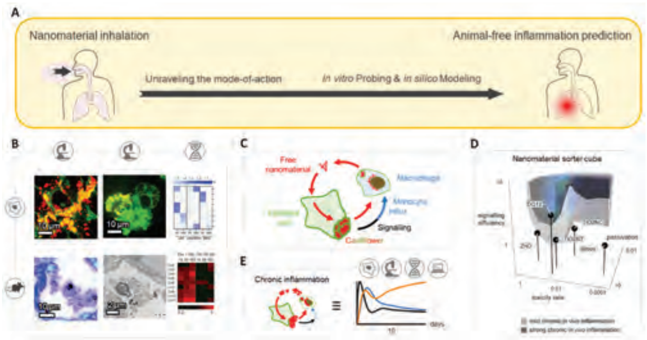

Figure 36: A) Development of the world's first animal-free prediction of chronic inflammation after nanoparticle inhalation: B) first, the mechanism of nanomaterial-induced inflammation was discovered using advanced microscopies and omics on in vitro and in vivo systems. C) The discovered events were causally connected into a network of events, shown here by a simplified scheme. D) Computer modelling of the network of events enabled classification of nanomaterials according to the predicted outcome of exposure based on three nanomaterial-specific parameters. E) By combining in vitro probing of these parameters and the in silico model, chronic inflammation can be predicted for any metal oxide nanomaterial in a time- and cost-efficient manner without animal testing.

Metamorphosis of the Carniolan bee (Apis mellifera carnica) monitored by MR microscopy

In cooperation with the Biotechnical Faculty (BF UL), we started studying the metamorphosis of the Carniolan bee with sequential MR microscopy in the summer of 2018. The study was demanding, as we had to provide the best conditions for the development of the bee inside the MR magnet during imaging, which lasted 14 days for an individual bee sample. We first isolated an individual cell with a larva and then imaged it until the emergence of an adult bee. During this time, approximately 80 three-dimensional images with a resolution of 80 micrometres were taken with a time interval of 4 hours. The recorded images were then segmented so that we could extract information on the temporal change in the volume of various organs (digestive tract, respiratory system, honey stomach, etc.). With the help of structural analysis of images using the grey-level cooccurrence matrix (GLCM) method, we were also able to determine the transformation of the flight muscle. To ensure the statistical significance of the results, imaging was performed on two bee samples. The results of MR images of bees were also verified by X-ray computed tomography that was taken at the department B1 at JSI, as well as with histological analysis performed by the BF UL. The results of this study were published in the article: Aleš Mohorič, Janko Božič, Polona Mrak, Kaja Tušar, Lin Chenyun, Ana Sepe, Urška Mikac, Georgy Mikhaylov, Igor Serša, "In vivo continuous three-dimensional magnetic resonance microscopy : a study of metamorphosis in Carniolan worker honey bees (Apis mellifera carnica)", *Journal of Experimental Biology*, Nov. 2020, vol. 223, iss. 21, DOI: 10.1242/jeb.225250.

A new method to improve the signal-to-noise ratio of MR images

We have developed a new method that can be used to improve the signal-to-noise ratio (SNR) in MR images. The method is based on the signal aliasing effect. This occurs in MR imaging when the imaging field of view (FOV) is smaller than the sample size. The phenomenon leads to artefacts of MR images in usual samples, as parts of the sample outside the FOV are fold over into the image, which can lead to their overlap with the image of the sample within the FOV. We found that for a special type of sample, i.e., for periodic samples, this undesirable phenomenon can be used for the constructive superposition of the aliased signals and thus for signal amplification without any noise increase, if these samples are imaged at FOV equal to the unit cell size of the periodic sample. The method was first theoretically analysed, then verified on a model sample in two dimensions, and finally the practical use of this method was demonstrated by the imaging of a periodic array of drug tablets with extremely low NMR signals due to the low moisture content in the tablets. There was not enough signal from a single tablet to be able to get its MR image. However, with the presented method, it was straightforward to obtain the image of the tablet. The results of this study were published in the article: Igor Serša, "Magnetic resonance microscopy of samples with translational symmetry with FOVs smaller than sample size", *Scientific reports*, 2021, vol. 11, 541-1-541-12, IDOI: 10.1038/s41598-020-80652-z.

Study of medial and ulnar nerve morphology

This study was initiated by our partners from the Institute of Anatomy (MF UL). In the study three radiological methods are compared according to their diagnostic potential for separating fine structures within individual nerve fibres. Nerve-fibre samples were isolated human medial and ulnar nerves, then they were imaged, and finally we wanted to pinpoint the number and size of individual fascicles from their images. The radiological methods used were clinical MR imaging at 3T (3T-MRI), high-resolution ultrasound imaging (HRUS), magnetic resonance microscopy (MRM) at 9.4 T. Images of these three methods were also compared with the reference histological analysis method. The results of the study showed that of all the three radiological methods, MRM imaging has the highest diagnostic potential, less efficient but still relatively good was HRUS, while 3T-MRI proved to be the worst. The results of this study were published in a leading journal in the field of radiology in the article: Žiga Snoj, Igor Serša, Urša Matičič, Erika Cvetko, Gregor Omejec, "Nerve fascicle depiction at MR microscopy and high-frequency US with anatomic verification", *Radiology*, 2020, vol. 297, no. 3, pp. 1-3, DOI: 10.1148/radiol.2020201910.

Development of MR contrast agents based on magneto-liposomes

We participated in the characterization of the MR properties of a new type of contrast agents developed by the department K7 at JSI. These contrast agents are based on superparamagnetic iron nanoparticles, which are incorporated into the bilayer membrane of liposomes for better biocompatibility and therapeutic possibilities, thus obtaining magneto-liposomes (MLs). In the study, we first measured the NMR relaxation properties of differently concentrated aqueous ML solutions. This was followed by experiments on a culture of healthy and cancerous (T24) urothelial cells, to which MLs were added at various concentrations. The cell-culture samples were MR imaged using the T2 mapping method. In the experiments, we showed that MLs accumulate more markedly in cancer cells, so the MR signal of these cells is much shorter (T2-NMR relaxation time is greatly shortened) and thus allows efficient separation between healthy and cancer cells. The results of this study are published in the article: Nina Kostevšek, Calvin Cheung, Igor Serša, Mateja Erdani-Kreft, Ilaria Monaco, Mauro Comes Franchini, Janja Vidmar, Wafa Al-Jamal, "Magneto-liposomes as MRI contrast agents: a systematic Study of different liposomal formulations", *Nanomaterials*, 2020, vol. 10, no. 5, pp. 889-1-889-18,DOI: 10.3390/nano10050889.

MR imaging study of controlled-release tablets

We studied the effect of different pH and mechanical stresses on the formation of a gel layer and on the release of pentoxifylline from xanthan tablets. The mechanical stress on the tablets was caused by a flow of liquid surrounding the tablets. A biomodal method was used for tablet testing. In it, MR imaging was used to monitor the formation of a gel layer and sampling of the liquid medium in which the tablet dissolved allowed us to monitor the release of the drug from the tablets. The obtained results showed that in the pH neutral medium (water) the structure of the gel layer is weaker and less resistant to erosion than the structure of the gel layer obtained in the acid medium. Different pH values of the medium also influenced the different mechanisms of drug release from the tablets. This was predominantly erosive in the case of a neutral medium and was diffusive in the case of an acidic medium. The effect of fluid flow around the tablets was important in the erosive release mode at neutral pH, while the effect of flow was negligible in the case of the diffusion release mode at acidic pH due to the increased compactness of the gel layer. The results of the study were published in the article: MIKAC, Urška, KRISTL, Julijana. Magnetic resonance methods as a prognostic tool for the biorelevant behavior of xanthan tablets. *Molecules*. 2020, vol. 25, no. 24, pp. 1-12, DOI: 10.3390/molecules25245871.

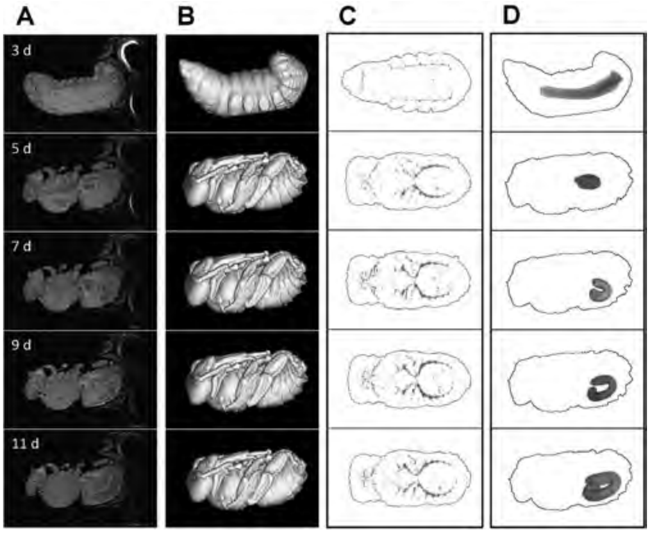

Figure 37: MR images of the metamorphosis of the Carniolan bee (Apis mellifera carnica) taken at two-day intervals: (A) T1-weighted MRI images from the 3D image set, (B) the corresponding volume rendered images, (C) the corresponding segmented respiratory system images, and (D) the corresponding segmented digestive tract images.

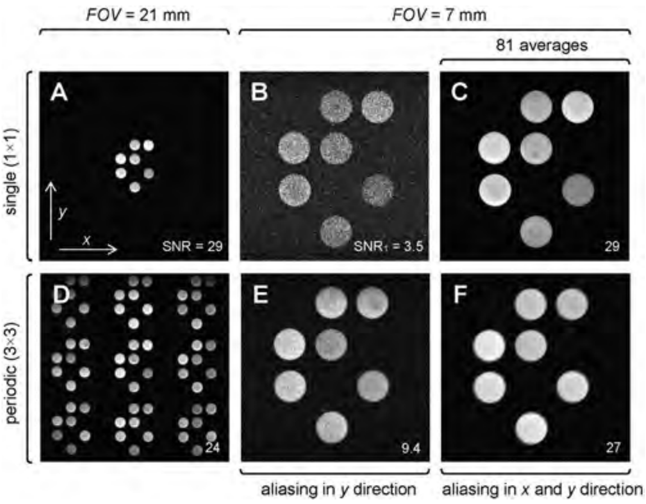

Figure 38: MR images of the test 2D periodic sample: (A-C) the sample consists only of the central object with the unit-cell dimension of 7 mm and (D-F) the sample consists of nine identical objects arranged in a 3 × 3 matrix. (A, D) When the central object was imaged at a field of view (FOV) equal to three times the unit-cell dimension, the SNR was nine times higher than in case (B) when this object was imaged at the FOV equal to the unit cell. When imaging a 2D periodic sample with the FOV equal to the unit cell, the SNR is increased relative to example (B) by a factor of: (E) three times when the constructive signal aliasing is present only in the phase direction and (F) nine times when the constructive signal aliasing is present along both axes of symmetry. (C) An image of the same SNR as in example (F) can also be obtained with 81 averages of the image signals of example (B).

The research in our department has been supported by a number of international projects financed by the European Union. It was also supported by many bilateral projects and other scientific cooperations. In 2020, the Department had cooperation with 113 partners from Slovenia and abroad. Among them were the following institutions:

1. BASF, Heidelberg, Germany
2. Ben Gurion University, Beersheba, Israel
3. Chalmers University of Technology, Physics Department, Göteborg, Sweden
4. Clarendon Laboratory, Oxford, Great Britain
5. Centre national de la recherché scientifique, Laboratory de Marseille, Marseille, France
6. Centre national de la recherché scientifique, Laboratoire de Spectrochimie Infrarouge et Raman, Thiais, France
7. Department of Chemistry, College of Humanities and Sciences, Nihon University, Tokyo, Japan
8. Deutsches Krebsforschungszentrum, Heidelberg, Germany
9. Deutsches Elektronen-Synchrotron, Hamburg, Germany
10. École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
11. Eidgenössische Technische Hochschule - ETH, Zürich, Switzerland
12. Elettra (Synchroton Light Laboratory), Basovizza, Italy

13. European Synchrotron Radiation Facility, Grenoble, France
14. Facultad de Ciencia y Technologia, Universidad del Pais Vasco UPV/EHU, Leioa, Spain
15. Faculty of Physics, Adam Mickiewicz University, Poznan, Poland
16. Florida State University, Florida, USA
17. Forschungszentrum Dresden Rossendorf, Dresden, Germany
18. Gunma National College of Technology, Maebashi, Japan
19. High-Magnetic-Field Laboratory, Grenoble, France
20. High Magnetic Field Laboratory, Nijmegen, the Netherlands
21. High Magnetic Field Laboratory, Tallahassee, Florida, USA
22. Humboldt Universität Berlin, Institut für Biologie/Biophysik, Berlin, Germany
23. Illie Murguescu Institute of Physical Chemistry of the Romanian Academy, Bucharest, Romania
24. International Human Frontier Science Program Organisation, Strasbourg, France
25. Institut Ruđer Bošković, Zagreb, Croatia
26. Institute for Theoretical Physics in Göttingen, Göttingen, Germany
27. Institute of Molecular Physics, Polish Academy of Sciences, Poznan, Poland
28. Institute of Electronic Materials Technology, Warsaw, Poland
29. Institut für Experimentalphysik der Universität Wien, Vienna, Austria
30. Institut für Biophysik und nanosystemforschung OAW, Graz, Austria
31. Institute for Crystallography, Russian Academy of Sciences, Moscow, Russia
32. Instituto Superior Tecnico, Departamento de Fisica, Lisbon, Portugal
33. International Center for Theoretical Physics, Trieste, Italy
34. ISIS, Rutherford Appleton Laboratory, Didcot, Great Britain
35. A.F. Ioffe Physico-Technical Institute, Saint Petersburg, Russia
36. Kavli Institute for Theoretical Physics, Santa Barbara, USA
37. King's College, London, Great Britain
38. Klinični center Ljubljana, Ljubljana, Slovenia
39. Korea Basic Science Institute, Daejeon, South Korea
40. Kyung Hee University of Suwon, Impedance Imaging Research Center, Seoul, South Korea
41. KTH Royal Institute of Technology, Stockholm, Sweden
42. KMZ - CNC obdelava kovin in drugih materialov Zalar Miran s.p., Ljubljana, Slovenia
43. Liquid Crystal Institute, Kent, Ohio, USA
44. Max Planck Institute, Dresden, Germany
45. Mayo Clinic, Rochester, Minnesota, USA
46. Merck KGaA, Darmstadt, Germany
47. MH Hannover, Hannover, Germany
48. National Academy of Sciences of Ukraine, Institute of Physics, Kyiv, Ukraine
49. National Center for Scientific Research "Demokritos", Aghia Paraskevi Attikis, Greece
50. National Institute for Research in Inorganic materials, Tsukuba, Japan
51. Nuklearni Institut Vinča, Beograd, Serbia
52. Oxford University, Department of Physics, Department of Materials, Oxford, Great Britain
53. Paul Scherrer Institut, Villigen, Switzerland
54. Politecnico di Torino, Dipartimento di Fisica, Torino, Italy
55. Radbound University Nijmegen, Research Institute for Materials, Nijmegen, the Netherlands
56. Rwth Aachen University, Aachen, Germany
57. School of Physics, Hyderabad, Andhra Prades, India
58. SISSA, Trieste, Italy
59. State College, Pennsylvania, USA
60. Sveučilište u Rijeci, Medicinski fakultet, Rijeka, Croatia
61. Sveučilište u Zagrebu, Institut za fiziku, Zagreb, Croatia
62. Technical University of Catalonia, Barcelona, Spain
63. Technical University Vienna, Vienna, Austria
64. The Geisel School of Medicine at Dartmouth, Hanover, USA
65. The Max Delbrück Center for Molecular Medicine in Berlin, Berlin, Germany
66. Tohoku University, Sendai, Japan
67. Tokyo University, Bunkjo, Tokyo, Japan
68. University of Aveiro, Aveiro, Portugal
69. Universita di Pisa, Dipartimento di Chimica e Chimica Industriale, Pisa, Italy

70. Université de Picardie Jules Verne, Amiens, France
71. Université de la Méditerranée, Marseille, France
72. University of Bristol, Bristol, Great Britain
73. University of California at Irvine, Beckman Laster Institute and Medical Clinic, Irvine, California, USA
74. University of Durham, Durham, Great Britain
75. University of Duisburg, Duisburg, Germany
76. University of Innsbruck, Innsbruck, Austria
77. Universität Freiburg, Institut für Makromolekulare Chemie, Freiburg, Germany
78. University of Linz, Institute of Chemistry, Department of Physical Chemistry & Linz Institute of Organic Solar Cells, Linz, Austria
79. University of Leeds, Leeds, Great Britain
80. University of Loughborough, Loughborough, Great Britain
81. Universit*ä*t Mainz, Geowissenschaften, Mainz, Germany
82. Université de Nice, Nice, France
83. Université Paris Sud, Paris, France
84. University of Provence, Marseille, France
85. University of Tsukuba, Tsukuba, Ibaraki, Japan
86. University of Utah, Department of Physics, Salt Lake City, Utah, USA
87. University of Waterloo, Department of Physics, Waterloo, Ontario, Canada
88. Universit*ä*t Regensburg, Regensburg, Germany
89. University of Zürich, Zürich, Switzerland
90. University of Munich and MPQ, Munich, Germany
91. University of Mons, Mons, Belgium
92. University of Pavia, Pavia, Italy
93. Universy of Maribor, Maribor, Slovenia
94. University of North Carolina at Chapel Hill, Chapel Hill, USA
95. University of Wisconsin–Madison, Madison, USA
96. Wagenigen University, Laboratory of Biopyhsics, Wageningen, the Netherlands
97. Weizman Institute, Rehovot, Israel
98. Yonsei University, Seoul, South Korea

that made the reported studies possible.

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. 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.
8. 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.
9. 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.
10. 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.

11. A. Hassanien, B. Zhou, A. Kobayashi. *Spontaneous Antiferromagnetic Ordering in a Single Layer of (BETS)$_2$GaCl$_4$ Organic Superconductor.* Advanced Electronic Materials **6** (2020).
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13. 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.
14. 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.

Some outstanding publications in 2019

1. M. Gomilšek, R. Žitko, M. Klanjšek, M. Pregelj, C. Baines, L. Yuesheng, Q. Zhang, A. Zorko, *Kondo screening in a charge-insulating spinon metal.* Nature Physics 15 (2019) 754.
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3. B. Senyuk, J. Aplinc, M. Ravnik, I. I. Smalyukh, High-order elastic multipoles as colloidal atoms. Nature Communications 10 (2019) art. no. 1825, doi: 10.1038/s41467-019-09777-8.
4. S. Čopar, J. Aplinc, Ž. Kos, S. Žumer, M. Ravnik, Topology of three-dimensional active nematic turbulence confined to droplets. Physical Review X 9 (2019) 031051-1-031051-13.
5. J. Pollard, G. Posnjak, S. Čopar, I. Muševič, G. P. Alexander. Point defects, topological chirality and singularity theory in cholesteric liquid-crystal droplets. Physical Review X 9 (2019) 021004-1-021004-19.
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Some outstanding publications in 2018

1. N. Janša, A. Zorko, M. Gomilšek, M. Pregelj, K.W. Krämer, D. Biner, A. Biffin, C. Rüegg, M. Klanjšek. Observation of two types of fractional excitation in the Kitaev honeycomb magnet. *Nature Physics* **14**, (2018), 786-790.
2. P. Adler, P. Jeglič, T. Knaflič, M. Komelj, D. Arčon, et al. Verwey-type charge ordering transition in an open-shell p-electron compound. *Science Advances* 4, (2018), eaap7581.
3. S. Gao, S. Vrtnik, J. Luzar, et al. Dipolar spin ice states with a fast monopole hopping rate in CdEr$_2$X$_4$ (X=Se, S). *Physical Review Letters* **120** (2018), 137201.
4. Yu.O. Zagorodniy, B. Zalar et al. Chemical disorder and ^{207}Pb hyperfine fields in the magnetoelectric multiferroic Pb(Fe$_{1/2}$Sb$_{1/2}$)O$_3$ and its solid solution with Pb(Fe$_{1/2}$Nb$_{1/2}$)O$_3$. *Physical Review Materials* **2** (2018), 014401.
5. J. Dolinšek. Electronic transport properties of complex intermetallics. *Crystal growth of intermetallics*, Eds. P. Gille, Yu. Grin (Berlin: De Gruyter, 2018), 260-278.
6. Pramanick, A., Dmowski, W., Egami, T.I, Setiadi Budisuharto, A., Weyland, F., Novak, N., Christianson, A., Borreguero, J. M., Abernathy, D., Jørgensen, M. R. V., Stabilization of Polar Nanoregions in Pb-free Ferroelectrics. *Physical Review Letters* **120** (2018), 207603.
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10. Santos, Ana Mafalda, Urbančič, Iztok, et al. Capturing resting T cells: the perils of PLL. *Nature Immunology* **19** (2018), 203-205.

Awards and Appointments

1. Dr Matjaž Gomilšek: Jožef Stefan Golden Emblem Prize for his doctoral thesis "Quantum spin liquids on geometrically frustrated kagome lattices", Ljubljana, Jožef Stefan Institute
2. Prof. Samo Kralj, PhD: the Zois Certificate of Recognition for important research achievements in the field of soft-matter physics, Ljubljana

Patents granted

1. Luka Drinovec, Griša Močnik, Photo-thermal interferometer, EP3492905 (B1), European Patent Office, 29. 04. 2020, US10768088 (B2), US Patent Office, 08. 09. 2020.

INTERNATIONAL PROJECTS

1. Small Services
   Dr. Polona Umek
2. Double-Beam Laser Interferometer Measurement
   Prof. Vid Bobnar
   Tdk Electronics Gmbh & Co Og
3. CROSSING - Crossing Borders and Scales - An Interdisciplinary Approach
   Prof. Janez Štrancar
   Helmholtz-zentrum Dresden-rossendorf E.v.
4. COST CA15209; European Network on NMR Relaxometry
   Prof. Tomaž Apih
   Cost Office
5. COST CA16109; Chemical On-Line Composition and Source Apportionment of Fine Aerosol
   Prof. Griša Močnik
   Cost Office
6. COST CA16218; Nanoscale Coherent Hybrid Devices for Superconducting Quantum Technologies
   Dr. Abdelrahim Ibrahim Hassanien
   Cost Association Aisbl
7. COST CA16221; Quantum Technologies with Ultra-Cold Atoms
   Dr. Peter Jeglič
   Cost Association Aisbl
8. COST CA17121; Correlated Multimodal Imaging in Life Sciences
   Prof. Janez Štrancar
   Cost Association Aisbl
9. COST CA17139; European Topology Interdisciplinary Action
   Prof. Slobodan Žumer
   Cost Association Aisbl
10. COST CA16202; International Network to Encourage the Use of Monitoring and Forecasting Dust Products
    Prof. Griša Močnik
    Cost Association Aisbl
11. COST CA9108 - HiSCALE; High-Temperature SuperConductivity for AcceLerating the Energy Transition
    Dr. Abdelrahim Ibrahim Hassanien
    Cost Association Aisbl
12. BIO-OPT-COMM; A Living Optically-Communicating Neural Network
    Asst. Prof. Matjaž Humar
    Hfspo- International Human Frontier
13. H2020 - SmartNanoTox; Smart Tools for Gauging Nano Hazards
    Prof. Janez Štrancar
    European Commission
14. H2020 - ENGIMA; Engineering of Nanostructures with Giant Magneto-Piezoelectric and Multicaloric Functionalities
    Prof. Zdravko Kutnjak
    European Commission
15. H2020 - Cell-Lasers; Intracellular Lasers: Coupling of Optical Resonances with Biological Processes
    Asst. Prof. Matjaž Humar
    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

RESEARCH PROGRAMMES

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

R & D GRANTS AND CONTRACTS

1. Sensor technologies in diagnostics and monitoring of cultural heritage buildings
   Prof. Janez Dolinšek
2. Electroporation-based treatments with new high-frequency electroporation pulses
   Prof. Igor Serša
3. Reconstruction of electrical conductivity of tissues by means of magnetic resonance techniques
   Prof. Igor Serša
4. Phase transitions towards coordination in multilayer networks
   Dr. Uroš Jagodič
5. Development of building blocks for new European quantum communication network
   Dr. Peter Jeglič
6. High-resolution optical magnetometry with cold cesium atoms
   Dr. Peter Jeglič
7. Integrated multi-channel artificial nose for vapor trace detection
   Prof. Igor Muševič
8. Photonic devices made entirely out of edible materials
   Asst. Prof. Matjaž Humar
9. Probing spin states near the surface of quantum spin materials
   Prof. Denis Arčon
10. Advanced soft nematocaloric materials
    Asst. Prof. Brigita Rožič
11. Multicaloric cooling
    Prof. Zdravko Kutnjak
12. Optimization of MRI techniques for assessment of thrombolytic treatment outcome
    Prof. Igor Serša
13. Intracellular lasers: Coupling of optical resonances with biological processes
    Asst. Prof. Matjaž Humar
14. Study of intracellular forces by deformable photonic droplets
    Asst. Prof. Matjaž Humar
15. Electrocaloric elements for active cooling of electronic circuits
    Prof. Vid Bobnar
16. Advanced inorganic and organic thin films with enhanced electrically-induced response
    Prof. Vid Bobnar
17. Adverse outcome pathway leading to atherosclerosis
    Dr. Tilen Koklič
18. Liquid-crystal microdroplet lasers for sensing inside live cells
    Zuhail Kottoli Poyil
19. Stabilization and destabilisation of spin liquids by perturbations
    Prof. Andrej Zorko
20. Physics of Majorana fermions in Kitaev magnets
    Dr. Martin Klanjšek
21. Novel experimental approach for determination of quantum spin liquids
    Prof. Andrej Zorko
22. Topological turbulence in confined chiral nematic fields
    Prof. Miha Ravnik
23. Controllable broadband electromagnetic-radiation shielding
    Dr. Matej Pregelj
24. Intelligent Content-Aware Nanospectroscopy (iCAN) of molecular events in nanoparticles-induced neurodegeneration
    Dr. Iztok Urbančič
25. Biopharmaceuticals: sensor for aggregation of protein particles based on liquid crystals
    Prof. Miha Ravnik
26. Spatial and temporal shaping of laser light for minimally invasive ophthalmic procedures
    Prof. Janez Štrancar
27. Domain engineered ferroelectric ceramic layer elements for efficient energy harvesting and energy conversion applications
    Prof. Zdravko Kutnjak
28. Magnetic, electric and stress – field programming of shape response in polymer-dispersed liquid crystal elastomers – based actuators
    Dr. Andraž Rešetič
29. Building blocks, tools and systems for the Factories of the Future – GOSTOP
    Prof. Janez Štrancar
    Ministry of Education, Science and Sport
30. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
    Prof. Igor Muševič
    Slovenian Research Agency

NEW CONTRACTS

1. 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.
2. Characterization of ferric carboxymaltose by atomic force microscopy
   Prof. Miha Škarabot
   Lek d. d.
3. Characterisation of iron-carboksimaltose with the electron paramagnetic resonance (EPR) technique
   Prof. Denis Arčon
   Lek d. d.
4. AerOrbi - Aerosol soft photo ionisation Orbitrap mass spectrometry
   Prof. Griša Močnik
   Aerosol d. o. o.

VISITORS FROM ABROAD

1. Hanani Zouhair, Cadi Ayyad University, Marrakesh, Morocco, 15 November 2019–15 January 2020
2. Dr Wencka Magdalena, Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland, 15 January–31 December 2020
3. Petrinović Toma, University of Zagreb, Institute of Physics, Zagreb, Croatia, 5–14 January 2020
4. Prof. Lancaster Tom, PhD, Durham University, Durham, United Kingdom, 12–17 January 2020
5. Dr Fukuda Jun-ichi, Kyushu University, Fukuoka, Japan, 12–18 January 2021
6. Dr Komitov Lachezar, University of Gothenburg, Gothenburg, Sweden, 2–7 March 2020
7. Dr Jampani Venkata Suba Rao, University of Luxembourg, Luxembourg, Luxembourg, 3 September–10 October 2020
8. Dr Višić Bojana, Institute of physics Belgrade, Belgrade Serbia, 1–10 October 2020
9. Nikolai Cyepurnyi, Ostbayerische Technische Hochschule Regensburg, Regensburg, Germany, 8–31 October 2020

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24. Asst. Prof. Dušan Ponikvar*
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27. Prof. Maja Remškar
28. Asst. Prof. Brigita Rožič
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30. Prof. Miha Škarabot
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68. Urška Gradišar Centa, B. Sc.
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98. Vesna Lopatič, B. Sc.
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101. Janja Milivojević
102. Ana Sepe, B. Sc.
103. Marjetka Tršinar

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Original Article

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2. Aurelien Barbotin, Iztok Urbančič, Silvia Galiani, Christian Eggeling, Martin J. Booth, "Background reduction in STED-FCS using a bi-vortex phase mask", *ACS photonics*, 2020, **7**, 7, 1742-1753.
3. Abdou Hassanien, Biao Zhou, Akiko Kobayashi, "Spontaneous antiferromagnetic ordering in a single layer of $(BETS)_2GaCl_4$ organic superconductor", *Advanced electronic materials*, 2020, **6**, 10, 2000461.
4. Rijeesh Kizhakidathazhath, Yong Geng, Venkata Subba R. Jampani, Cyrine Charni, Anshul Sharma, Jan P. F. Lagerwall, "Facile anisotropic deswelling method for realizing large-area cholesteric liquid crystal elastomers with uniform structural color and broad-range mechanochromic response", *Advanced functional materials*, 2020, **30**, 7, 1909537.
5. Hana Kokot *et al.* (34 authors), "Prediction of chronic inflammation for inhaled particles: the impact of material cycling and quarantining in the lung epithelium", *Advanced materials*, 2020, **32**, 47, 2003913.
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11. Itir Bakis Dogru-Yuksel, Mertcan Han, Gregor Pirnat, Emir Salih Magden, Erkan Senses, Matjaž Humar, Sedat Nizamoglu, "High-Q, directional and self-assembled random laser emission using spatially localized feedback via cracks", *APL photonics*, 2020, **5**, 10, 106105.
12. Rok Podlipec, Jaka Mur, Jaka Petelin, Janez Štrancar, Rok Petkovšek, "Two-photon retinal theranostics by adaptive compact laser source", *Applied physics. A, Materials science & processing*, 2020, **126**, 6, 405.
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15. S. Vratolis *et al.* (18 authors), "Comparison and complementary use of *in situ* and remote sensing aerosol measurements in the Athens Metropolitan Area", *Atmospheric environment*, 2020, **228**, 117439.
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44. Zouhair Hanani *et al.* (14 authors), "Enhanced dielectric and electrocaloric properties in lead-free rod-like BCZT ceramics", *Journal of advanced ceramics*, 2020, **9**, 2, 201-219.
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58. Jin Hyun Chang, Christian Baur, Jean-Marcel Ateba Mba, Denis Arčon, Gregor Mali, Dorothea Alwast, R. Jürgen Behm, Maximilian Fichtner, Tejs Vegge, Juan Maria Garcia-Lastra, "Superoxide formation in Li_2VO_2F cathode material - a combined computational and experimental investigation of anionic redox activity", *Journal of materials chemistry. A, Materials for energy and sustainability*, 2020, **8**, 32, 16551-16559.
59. Zouhair Hanani *et al.* (12 authors), "Structural, dielectric, and ferroelectric properties of lead-free BCZT ceramics elaborated by low-temperature hydrothermal processing", *Journal of materials science. Materials in electronics*, 2020, **31**, 13, 10096–10104.
60. Soukainae Merselmiz *et al.* (14 authors), "Enhanced electrical properties and large electrocaloric effect in lead-free $Ba_{0.8}Ca_{0.2}Zr_xTi_{1-x}O_3$ ($x = 0$ and 0.02) ceramics", *Journal of materials science. Materials in electronics*, 2020, **31**, 19, 17018–17028.
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1. Lina Boljka *et al.* (37 authors), *Bela knjiga o strokovnem varovanju okolja*, Institut "Jožef Stefan", 2020.

University, Higher Education or Higher Vocational Education Textbook

1. Simon Čopar, Daniel Svenšek, Aleš Mohorič, Saša Prelovšek, *Rešene kolokvijske naloge iz klasične fizike*, Fakulteta za matematiko in fiziko, 2020.
2. Andrej Zorko, Miha Nemevšek, Nejc Košnik, Matic Lubej, *Rešene naloge iz moderne fizike*, Fakulteta za matematiko in fiziko, 2020.

Secondary and Primary School Textbook or Other Textbook

1. Aleš Mohorič, Vito Babič, *Fisica 1: libro di testo di fisica per la prima classe del ginnasio e per gli istituti professionali*, Mladinska knjiga, 2020.
2. Aleš Mohorič, Vito Babič, *Fizika 2: učbenik za fiziko v 2. letniku gimnazij in štiriletnih strokovnih šol*, Mladinska knjiga, 2020.
3. Aleš Mohorič, Vito Babič, *Fizika 3: učbenik za fiziko v 3. letniku gimnazij in štiriletnih strokovnih šol*, Mladinska knjiga, 2020.

Patent Application

1. Roman Šink, Ema Valentina Brovč, Stane Pajk, Janez Mravljak, *Stabilization of pharmaceutical compositions comprising polysorbate*, EP3714902 (A1), European Patent Office, 30. 09. 2020.

Patent

1. Luka Drinovec, Griša Močnik, *Photo-thermal interferometer*, EP3492905 (B1), European Patent Office, 29. 04. 2020; US10768088 (B2), US Patent Office, 8. 09. 2020.

Theses and Mentoring

1. Tilen Knaflič, *Quantum magnetism in π-electron molecular systems:* doctoral dissertation, Ljubljana, 2020 (mentor Denis Arčon).
2. Jože Luzar, *Design and properties of lime-cement structural injection grouts for strengthening of heritage buildings:* doctoral dissertation, Ljubljana, 2020 (mentor Janez Dolinšek).
3. Luka Pirker, *Electrical, optical and structural properties of low-dimensional materials based on tungsten:* doctoral dissertation, Ljubljana, 2020 (mentor Maja Remškar).
4. Anja Pusovnik, *Flow of light in metamaterials based on nematic fluids:* doctoral dissertation, Ljubljana, 2020 (mentor Miha Ravnik).
5. Mitja Zidar, *Analysis and prediction of aggregation and degradation in protein-based biopharmaceuticals:* doctoral dissertation, Ljubljana, 2020 (mentor Miha Ravnik).

LABORATORY OF GASEOUS ELECTRONICS F-6

The research activities within the Department of Gaseous Electronics cover a variety of 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

Department F6 is a new research unit at the JSI, established in 2019. The major activities in 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 in 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 the grand challenges in science and technology as well as to support new, emerging fields of research.

From decoding of the mechanisms involved in the plasma-mediated degradation of mycotoxins to a step closer to the actual use of atmospheric pressure plasma technology as a new tool for the decontamination of mycotoxins. In 2020, Department F6 continued to explore the area of problems related to the global contamination of food with mycotoxins, emphasising the search for new solutions. As it has been shown in the past that cold plasma at atmospheric pressure (CAP) could be used as an effective tool against mycotoxins such as aflatoxins, trichothecenes, fumonisins and zearalenone [Toxins 11 (2019) 219] and for the successful inactivation of the mycotoxigenic mould Aspergillus flavus [Environmental Science & Technology 53 (2019) 1893-1904]. In 2020, we extended this research to the investigation of the mechanisms involved in plasma-induced degradation. This involved a model study using the air surface barrier discharge system (SBD), which was applied to degrade the mycotoxin aflatoxin B_1 (AFB_1), considered to be one of the most potent natural carcinogens [Journal of Hazardous Materials 403 (2020) 123593]. As already exposed in previous research, the plasma treatment led to the complete degradation of AFB_1 in less than 120 s of exposure. The efficacy of the CAP was compared to commercially used UV-C light irradiation. It was demonstrated that a plasma treatment led to significantly better decontamination of AFB_1, while UV-C irradiation led to only a 36% reduction of the initial AFB_1 concentration, even after the longest exposure time (480 s). Based on the data obtained from optical emission spectroscopy (OES) in Fourier-transformed infrared spectroscopy (FTIR) measurements, it was revealed that CAP produced reactive oxygen and nitrogen species (RONS) were crucial in the CAP decontamination processes. Using sophisticated analytical methods such as high-resolution mass spectrometry (HRMS) and nuclear magnetic resonance, it was indicated that plasma-induced degradation of the AFB_1 molecule initiated through the double bond between the C8 and C9 carbon atoms. This site is also responsible for the toxic effects of AFB_1. Further degradation continued through several different pathways and led to the formation of four key degradation products, which were, as AFB_1, completely decomposed or remained in traces after longer exposure times. The study also examined their cytotoxicity and genotoxicity using MTS and comet assay, respectively, which were performed in vitro with a Hep G2 cell culture. The viability of Hep G2 cells exposed to plasma-treated AFB_1 was not reduced and was comparable to the one observed in the control non-exposed group. Moreover, a significant decrease in DNA strand breaks was observed for samples exposed to CAP-treated AFB_1 samples, which corresponded to the values obtained from the controls. Thus, this research provides a key insight into CAP technology as a new decontamination tool and represents the first step towards applying the method for commercial purposes in the future.

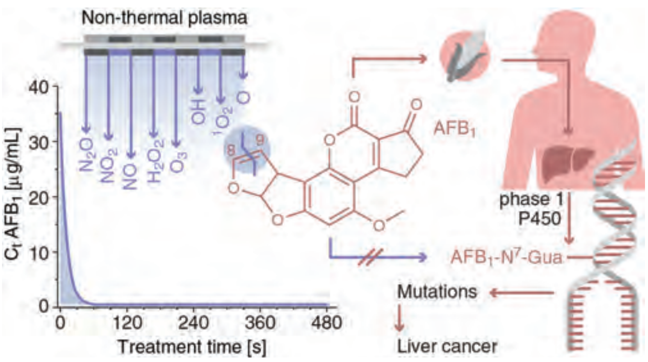

Figure 1: CAP degradation of mycotoxin AFB_1 and determination of the mechanisms involved in this process.

Figure 2: Dr Nataša Hojnik working on the research of fungi and mycotoxin plasma removal.

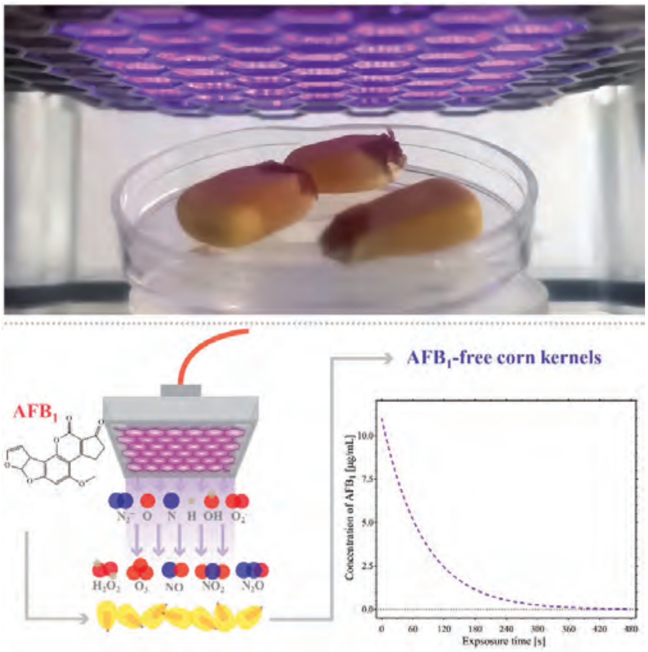

Figure 3: Decontamination of AFB$_1$ from corn kernels using CAP.

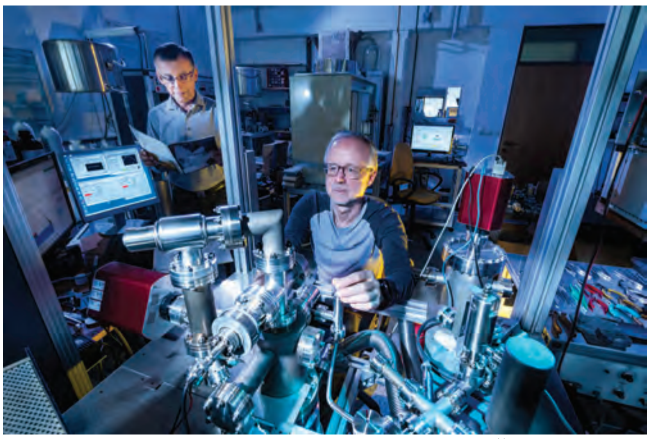

Figure 4: Researchers Dr Vincenc Nemanič and Marko Žumer running an experiment with thermal desorption in ultra-high vacuum.

Furthermore, the efficacy of plasma decontamination of AFB$_1$ was researched on real substrates – corn kernels [Plasma processes and polymers 18, 1 (2020), 2000163]. After applying the same discharge and experimental conditions as in the previous case, it was demonstrated that CAP treatment led to the successful removal of AFB$_1$, which was artificially applied to the surface of the corn kernels. This was followed by a detailed analysis of the potential plasma-induced modifications in the corn kernel surface's chemical composition, using techniques such as FTIR, X-ray photoelectron spectroscopy (XPS), contact-angle measurements and secondary ion mass spectroscopy (SIMS). As revealed by the results, the CAP treatment induced minor changes in the treated samples, indicating that indirect CAP treatments induced slight oxidation of the corn kernel surface. In addition, the potential plasma-induced morphological changes were examined as well. The results obtained from scanning electron microscopy (SEM) and atomic force microscopy (AFM) did not demonstrate any differences between the treated and non-treated samples. Hence, this study further proves that CAP technology represents a new, effective and safe approach to food processing and offers an immense improvement in terms of the scientific and technological levels.

Fusion research and understanding the interactions of hydrogen isotopes with fusion-related materials. The department researchers are members of the EUROfusion consortium, which works in fusion-related research following the current plan to confirm the operational principle towards the first fusion-power plant. Within the EUROfusion, our current research program focuses on the interactions of hydrogen isotopes with 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 from research and experiments that can be performed with hydrogen and deuterium, as they are all chemically similar. Much of the research thus flows with the three basic metals that make up the fusion reactor: tungsten, beryllium and austenitic low-carbon stainless steel of ITER quality. Using thermal desorption spectroscopy (TDS), we investigated in more detail the retention of tritium in the Be layers deposited on the walls in fusion reactors [Fus. Eng. Des. 150 (2020) 111365]. The interaction of hydrogen with tungsten oxides is completely unexplored, which is a relevant detail in the event of a sudden intrusion of air into the reactor in the case of an accident. The hot tungsten of the divertor would react violently with oxygen, but we cannot assess whether the resulting tritium oxide is porous or a barrier. In an original experiment, we measured the hydrogen permeation through a thin layer of tungsten on Eurofer before and immediately after oxidation. We have shown that tungsten oxide is highly inhibitory, a desirable property that can slightly inhibit the passage of tritium into the cooling system. [Journal of Nuclear Materials, 548 (2021) 152860].

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 liquid divertor was explored in recent years. The liquid metal trapped in the tungsten porous support structure continuously dissipates 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 the tin oxide. Our research demonstrated that tin itself is completely inert to deuterium since we could detect it only at an extremely low concentration, ~ 1 ppb D / Sn. [Nuclear fusion 21 (2021), 026009-1-026009-7].

Our atom-scale investigations of periodic and incommensurable crystal structures are giving us a unique insight into the very fundamental mechanisms of mechanical, magnetic, electrical, optical and thermal properties of metals, oxides, electronic ceramics and semiconductors. In addition to the investigations of ordered crystal structures and structural defects, our special focus is devoted to an investigation of the atypical surfaces and extrinsic states resulting from: i) defective surfaces where the translational symmetry of the surface is broken, ii) surfaces with adsorbed molecules, iii) interfaces between materials, e.g., semiconductor-oxide or semiconductor-metal, and iv) solid-liquid contact. Investigations of these conditions and phenomena are possible using the state-of-the-art research equipment available to researchers at the JSI, as well as in collaboration with the international research community.

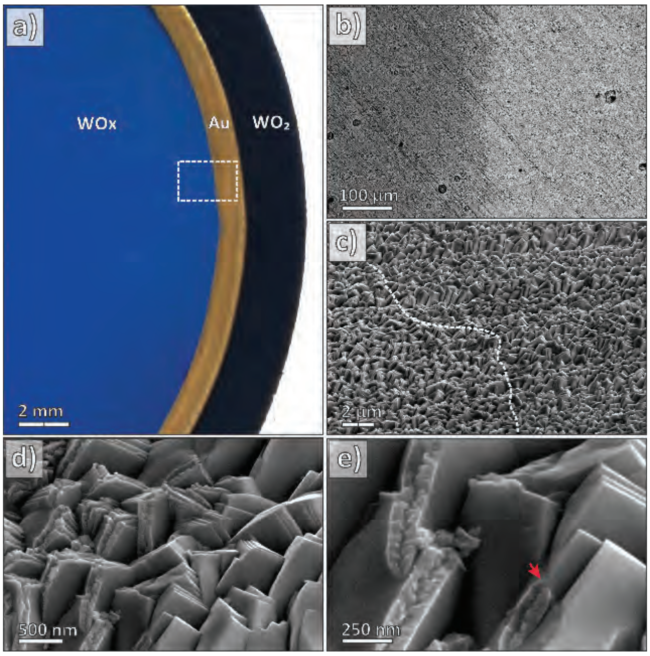

Figure 5: Surfaces of oxidized tungsten during hydrogen interaction experiment.

In the past year, our experimental findings were summarised in research articles on several different topics. In the field of condensed matter (materials, metals and semiconductors), we explored, by utilising photogrammetry, electron microscopy, electron crystallography, and molecular dynamic simulations, the nucleation and crystallisation mechanism of the metallic glass induced by high-energy laser irradiation [Applied Surface Science 505, 2020]. In the exploration of in-situ Ge quantum dots formation and their semiconducting properties, we combined grazing incidence X-ray diffraction, Raman spectroscopy, electron microscopy and grazing-incidence small-angle X-ray scattering [Vacuum 179, 2020].

The deposition, modification and analysis of the nanoparticles is also an important part of the functionalisation of the nanomaterials for the sensor applications. Such examples are screen-printed electrodes made of a mixture of plasmonic NPs in combination with glassy carbon for the detection of toxic algae [Biosensors & Bioelectronics 154, 2020] or the detection of bacteria [Sensors 20, 2020]. Similar nano-tailored electrodes were also proposed for the fast and accurate quality control for the detection of hydroquinone (HQ) and other phenolic compounds [Microchemical Journal 152, 2020].

Furthermore, we have demonstrated that the bulk optical, structural, and electronic properties of non-perovskite ferroelectrics can be fine-tuned by post-synthesis tailoring. For the first time, we performed the successful post-synthesis incorporation of metal dopants at elevated temperature into a host structure of $Sn_2P_2S_6$, known as the grandfather of dichalcogenide ferroelectrics, with the formula $M_2P_2X_6$ (M = metal and X = chalcogen). With the example of Cu, we show that the integration of dopant atoms into the bulk of an already-grown crystal could be easily tuned up to 0.5 at%, affecting the structural, optical, vibrational, electrical, and ferroelectric properties. Thermally diffused copper atoms in a $Sn_2P_2S_6$ bulk are in the metallic state, inducing a multiaxial expansion of the $Sn_2P_2S_6$ unit cell by 2–3.4%. The energy reduction between the indirect and direct optical transitions was observed, combined by small hardening for acoustic and soft optical vibrational modes originating in the partial substitution of Sn by Cu in the $Sn_2P_2S_6$ crystal lattice. Similar to hydrostatic pressure, the structurally bonded copper initiates a small downward shift in the critical temperature T_c. The presence of copper has a substantial impact on the shape smearing of the ferroelectric domains as well as on the behaviour of the dielectric permittivity. The real part of the dielectric constant ε′ reaches its maximum value at intermediate concentrations of Cu 0% < x < 0.5%, showing a ~20% increase with respect to the parent structure. The incorporated metal atoms provoke a monotonous expansion of the ferroelectric P–E loops along the increased dopant content direction. An increase in the electrical conductivity at higher Cu concentration reveals a trend for inducing metal-like behaviour.

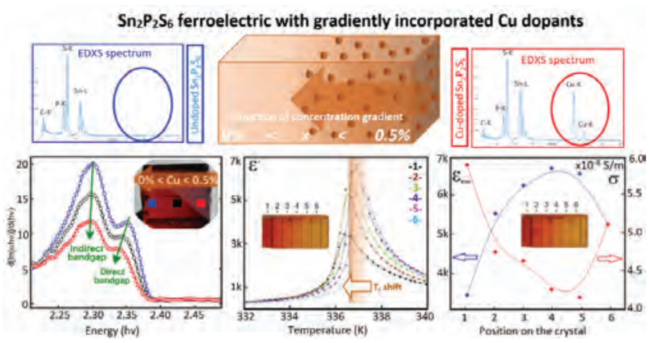

Figure 6: $Sn_2P_2S_6$ ferroelectric with gradiently incorporated Cu dopants.

Research in this domain was also attributed to the control and design of oxygen vacancies in nanomaterials, which can enable material-properties tuning. This was demonstrated for photoluminescence modifications in the case of tungsten oxide nanomaterials. Sub-stoichiometric tungsten oxide (WOx, 2 < x < 3) nanomaterials are important nanoscale semiconductor materials with broad applications in optoelectronic devices; however, a controllable modification of their physical properties remains challenging task. Here, we report an alternative green synthesis of hybrid nanostructures composed of the WOx and $ZnWO_4$ phases in ethanol via a solvothermal process using ZnO and WCl_6 as the precursors. The results indicate that the formation of $ZnWO_4$ leads to the structural conversion of WOx from nanorods to nanoparticles due to the effect of $ZnWO_4$ on the side growth of WOx nanostructures. Moreover, the surface morphology tailored by $ZnWO_4$ and crystalline phase transformation induces different photoluminescence (PL) emission from pure WOx nanostructures and WOx/$ZnWO_4$ hybrid nanostructures due to the increased number of oxygen vacancies.

Designing plasmonic surfaces with plasma processing. Nanoplasmonics have significant potential in novel analytical sensors for the fast and reliable recognition of analytes in ppm quantities. Today, there are several well-established research directions where plasmonic detection is employed extensively, i.e., food and water quality monitoring, viruses, pathogenic bacteria and hazardous toxin investigations for theranostic applications, and explosive substance detection for military and civil protection purposes. A combination of vibrational spectroscopy and surface nanoengineering has gained a reputation as a powerful weapon for the rapid and accurate determination of sub-molecular quantities of analytes. Signal enhancement achieved by employing various metallic nanoparticles and nanostructures can be amplified significantly due to the electromagnetic field confinement effect. Localised surface plasmon waves, which are responsible for the phenomenon, promote light absorption at nanovolume, generating 'hot spots' with an incredibly intense and confined electromagnetic field close to the nanosculptured metallic surface. However, the formation of the hot spot network is heavily dependent on the morphology, size, and spatial arrangement of plasmonic nanomaterials. Under optimal excitation conditions, the interaction between the optically induced electromagnetic field in the hot spot region and a probing analyte attached to the nanosculptured metallic substrate enlarges the photon scattering cross-section, increasing signal intensity by 10^6–10^{10}. As a result, fast single-molecule vibrational fingerprint recording is possible. Our focused review collected the recent state-of-the-art developments in nanoplasmonic SERS sensing, highlighting the most efficient surface morphology designs [Applied Physical Reviews, 7(3), 031307, 2020].

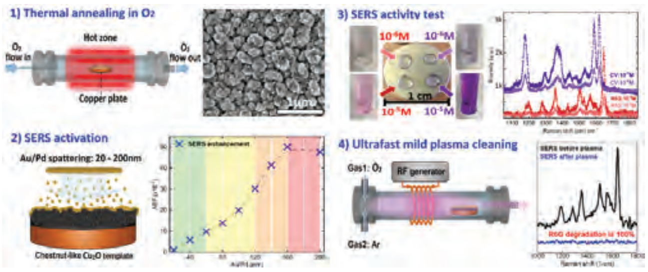

Figure 7: Schematic of the protocol for the preparation and testing of plasmonic surfaces.

Generally, the optical performance of the plasmonic substrate depends heavily on surface morphology specifications. Therefore, reliable and reusable plasmonic substrates are crucial for the development of biosensing applications using surface-enhanced Raman scattering (SERS), as they can provide unique advantages for the ultrafast and accurate single-molecule recognition of different species. These properties are unrevealed in this paper, where thermally annealed cupric CuO and cuprous oxide Cu_2O heterostructures were used as templates for highly stable nanotextured surfaces and the design of robust 3D plasmonic biochips. Differently tailored nano/micro-roughness provided outstanding light-trapping abilities that lead to significant SERS performance improvement. It was found that the Cu_2O chestnut-like substrate activated with 80-nm Au/Pd alloy film reveals an impressive 3.7-fold Raman signal increment in respect to the grainy-like structure and an about twice larger amplification than that of nanowires enriched platform decorated in the same manner. A large enhancement factor AEF ~5×10^5 of a chestnut-like Au/Pd@/Cu_2O chip allows adding it to the list of the most effective oxide-based plasmonic substrates. Moreover, the substrate shows unprecedented durability during repetitive plasma-cleaning, demonstrating a remarkable 100% self-recovery in less than 1 min, accompanied by virtually no thickness degradation of the plasmonic layer.


Figure 8: PhD student Neelakandan M. Santosh during the operation of atmospheric pressure plasma deposition.

The department F6 continued the research and development of atmospheric pressure plasmas. The research was done for water treatment, biological applications, and also for nanostructuring surfaces. In this year, we have developed and optimised an atmospheric plasma jet synthesis and deposition technique for metal-oxide nanoparticles. In the general interest of F6 into batteries and supercapacitors, we have focused on vanadium pentoxide (V_2O_5). This transitional metal-oxide is highly desirable in certain fields of industry, especially in catalysis, energy materials, medicine and aerospace, due to its optoelectronic properties, and it is predicted that its use will only increase in the coming decade. The developed technique enables the production of pure crystalline nanoparticles by conversion of macropowder of the same compound. The resulting metal-oxide nanoparticles are unimodal and are deposited on a selected substrate during the synthesis. The powder reform to nanoparticles is done at low temperature. Thus, the substrates can also be temperature-sensitive, like plastic. The method is effective, simple and offers a control over the purity and crystallinity of nanoparticles. This makes it very innovative and industry-applicable.

Enabling the synthesis of graphene and hybrid nanomaterials for energy-storage applications. Another research achievement from the nanotechnology field was the low-pressure plasma synthesis of hybrid Ni_3S_2@carbon nanostructures on metal substrates. In the researched case, carbon nanotubes were grown on a nickel substrate. During their growth, a piece of nickel, a nanoparticle, is transported from the substrate to the top of each nanotube. As nickel is a good catalyst, this has opened the doors to a lot of electrochemical applications. We have limited our interests to use the samples as electrodes in batteries and supercapacitors. In addition, the carbon nanotubes grew directly from a nickel substrate, which guaranteed a good electrical contact, the density of nanotubes was high, and with it, a large surface area was assured. However, the electrochemical tests for the application in Li-ion batteries were not impressive. Thus, we have added a thermal treatment of the samples in H_2S gas. A Ni_3S_2 layer formed on the nickel nanoparticles on top of carbon nanotubes. The morphology was "broccoli-like", which meant that the surface area further increased, and due to the chemical properties of nickel sulphide, the electrode became much more stable. As a battery electrode, that meant high reversible capacity, long-term cycling stability and high reversible capacity at high current densities.

A similar approach was taken for the preparation of electrodes for the supercapacitors. The same low-pressure plasma synthesis was used for carbon nanotubes with a nickel nanoparticle top. An alternate path was then taken by additional nitrogen-containing plasma modification of the electrode – nickel was shelled by a thin single-crystal nickel nitride (Ni_3N) layer. This layer completely changed the dynamic of the sulphurisation step that followed. In this case a smooth crystalline layer of Ni_3S_2 was created on the top. Based on the electrochemical measurements, the hybrid binder-free electrode exhibits one of the best electrochemical performance among Ni_3S_2 based electrodes with ultra-high specific capacity (856.3C g^{-1} at 3 A g^{-1}), outstanding rate capability (77.5 % retention at 13 A g^{-1}) and excellent cycling stability (83 % retention after 4000 cycles at 13 A g^{-1}), which is one of the best at the moment (Fig. 9, bottom). This means that capacitors made of this electrode would have a high capacity for electric energy storage, they would charge and discharge at high electric current density and would survive countless charge-discharge cycles.

The developed methods were patented, and their scientific aspects were published or are submitted for publications to leading scientific journals in the field. The batteries and supercapacitors for energy storage are immensely important for the transition to renewable energy sources and green technology, which we are performing with the H2020 FET-Open project "Pegasus".

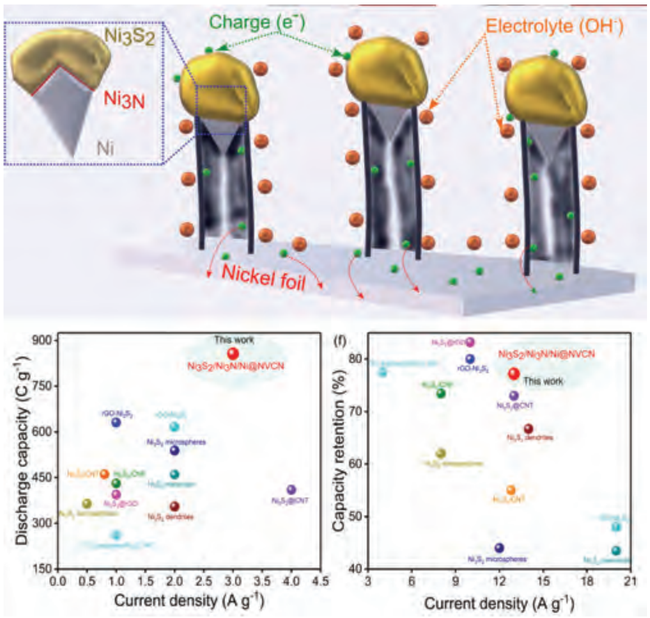

Figure 9: Schematic presentation of the $Ni_3S_2/Ni_3N/Ni@NVCN$ as an advanced electrode material for supercapacitors (top); comparison of specific capacity of Ni_3S_2-based electrodes with $Ni_3S_2/Ni_3N/Ni@NVCN$ (bottom-left) and comparison of rate capability performances of Ni_3S_2-based electrodes with $Ni_3S_2/Ni_3N/Ni@NVCN$.

Some outstanding publications in the past year

1. Vasyl Shvalya, Gregor Filipič, Janez Zavašnik, Ibrahim Abulhalim, Uroš Cvelbar. "Surface-enhanced Raman spectroscopy for chemical and biological sensing using nanoplasmonics: The relevance of interparticle spacing and surface morphology", *Applied Physics Reviews*, *7*(3), 031307, 2020.
2. Neelakandan Marath Santhosh, Gregor Filipič, Eva Kovačević, Andrea Jagodar, Johannes Berndt, Thomas Strunskus, Hiroki Kondo, Masaru Hori, Elena Tatarova, Uroš Cvelbar. N-graphene nanowalls via plasma nitrogen incorporation and substitution: the experimental evidence. *Nano-micro letters*. vol. 12, no. 1, str. 53-1-53-17. ISSN 2311-6706, 2020.
3. Vasyl Shvalya, Gregor Filipič, Damjan Vengust, Janez Zavašnik, Martina Modic, Ibrahim Abdulhalim, Uroš Cvelbar. "Reusable Au/Pd-coated chestnut-like copper oxide SERS substrates with ultra-fast self-recovery", *Applied Surface Science*, *517*, 146205, 2020.
4. N. Bundaleska, Janez Zavašnik, Uroš Cvelbar, et. al. Prospects for microwave plasma synthesised N-graphene in secondary electron emission mitigation applications. *Scientific reports*. 2020, vol. 10, str. 13013-1-13013-13. ISSN 2045-2322. DOI: 10.1038/s41598-020-69844-9.
5. Vincenc Nemanič, Marko Žumer, Corneliu Porosnicu, B. Butoi, E. Alves, R. Mateus. Deuterium inventory determination in beryllium and mixed beryllium-carbon layers doped with oxygen. *Fusion engineering and design*. [Print ed.]. 2020, vol. 150, str. 111365-1-111365-7. ISSN 0920-3796.

6. Xinyu Song, Uroš Cvelbar, Petra Stražar, Lutz Vossebein, Andrea Zille. Antimicrobial efficiency and surface interactions of quaternary ammonium compound absorbed on Dielectric Barrier Discharge (DBD) plasma treated fiber-based wiping materials. *ACS applied materials & interfaces*. 2020, vol. 12, no. 1, str. 298-311. ISSN 1944-8244. DOI: 10.1021/acsami.9b18746
7. Vasyl Shvalya, Janez Zavašnik, Venera Nasretdinova, Hana Uršič Nemevšek, Janez Kovač, Alexander A. Grabar, Anton A. Kohutych, Alex Molnar, Dean R. Evans, Dragan Mihailović, Uroš Cvelbar. "Customisation of Sn2P2S6 ferroelectrics by post-growth solid-state diffusion doping ", *Journal of Materials Chemistry C*, *8*(29), 9975-9985, 2020.

Organization of conferences, congresses and meetings

1. Organization of the workshop "Gaseous Electronics Symposium – GES3", Rogla, 2–6 February 2020

Patent granted

1. Metod Kolar, Miran Mozetič, Ita Junkar, Alenka Vesel, Martina Modic, Karin Stana-Kleinschek, Method for immobilization of heparin on a polymeric material, EP2997984 (B1), European Patent Office, 03. 06. 2020.

INTERNATIONAL PROJECTS

1. COST CA15114; Anti-Microbal Coating Innovations to prevent Infectious Diseases (AMICI)
   Prof. Uroš Cvelbar
   Cost Office
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. H2020 - PEGASUS; Plasma Enabled and Graphene Allowed Synthesis of Unique nano Structures
   Prof. Uroš Cvelbar
   European Commission
6. H2020 - EUROfusion; Plasma Facing Components-1-IPH-FU, EUROfusion
   Dr. Vincenc Nemanič
   European Commission
7. H2020 - EUROfusion; WPPFC-PEX-FU, WPPFC-PEX-FU, EUROfusion
   Dr. Vincenc Nemanič
   European Commission
8. Investigation of Helium Retention in Plasma Facing Materials Using Advanced Analytical Methods
   Asst. Prof. Janez Zavašnik
   Slovenian Research Agency
9. Oxidative Stress Responses of Microbial Biofilms Exposed to Cold Atmospheric Pressure Plasma Generated Reactive Species
   Dr. Martina Modic
   Slovenian Research Agency
10. Designing Catalytic Activity of Nanomaterials with Plasma
    Prof. Uroš Cvelbar
    Slovenian Research Agency
11. Beyond Graphene - The New Materials based on 2D and 3D Graphene
    Prof. Uroš Cvelbar
    Slovenian Research Agency
12. Exploration of Metal/Metal-Oxide Sensor Capabilities
    Dr. Gregor Filipič
    Slovenian Research Agency

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-assisted wound treatment and topical introduction of molecules
   Prof. Uroš Cvelbar
2. Novel higly sensitive and fast water qulity monitoring sensors
   Prof. Uroš Cvelbar
3. Plasma In-situ reactions and single crystal Transitions
   Prof. Uroš Cvelbar
4. Hybrid and Reengineered Nanocatalysts for New Purification Routes
   Prof. Uroš Cvelbar
5. Plasma decontamination of mycotoxins and inactivation of fungi in food industry
   Dr. Martina Modic
6. Selective plasma oxidation of FeCrAl alloys for extended-lifetime of glow plugs for diesel engines
   Dr. Vincenc Nemanič
7. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
   Prof. Uroš Cvelbar
   Slovenian Research Agency

VISITOR FROM ABROAD

1. Ivana Sremački, University of Ghent, Belgium, 16 June to 18 July 2020

STAFF

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4. Vasyl Shvalya, B. Sc.
5. Asst. Prof. Janez Zavašnik

Postdoctoral associates
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7. Dr. Nataša Hojnik

Postgraduates
8. Martin Košiček, B. Sc.
9. *Petra Stražar, B. Sc., left 01.11.20*
10. Marko Žumer, B. Sc.

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

Technical and administrative staff
13. *Ula Groznik, B. Sc., 01.04.20, transferred to Department F7*
14. Urška Kisovec, B. Sc.

BIBLIOGRAPHY

ORIGINAL ARTICLE

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DEPARTMENT FOR COMPLEX MATTER F-7

The research within the Department of Complex Matter encompasses a variety of research fields, ranging from fundamental investigations of elementary excitations in quantum materials, non-equilibrium 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 syntheses. Our research into ultra-fast, non-equilibrium transitions, investigations of new emergent hidden orders and ferromagnetic liquids are of significant interest worldwide.

Head:
Prof. Dragan D. Mihailović

European Research Council
Established by the European Commission

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

The experimental research within the department is strongly supported by theory, with approaches 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 ultra-fast, low-energy, cryo-memory devices based on our studies of ultra-fast electronic transitions.

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

Charge Configuration Memory devices

Superconducting electronics and quantum technologies could prove to lead the next generation of computing; however, their progress is slowed by the absence of a suitable memory device that would be energy efficient, ultra-fast, non-volatile and operate at cryogenic temperatures. We propose a novel type of a memory device to satisfy these requirements based on resistance switching between different charge ordered states in a transition-metal dichalcogenide 1T-TaS_2. Such Charge Configuration Memory (CCM) devices can operate down to temperatures of 250 mK, can be scaled down to a few tens of nanometres in dimensions and can withstand more than 10 million switching operations. CCM devices can also be triggered using picosecond pulses, so they can be coupled and used in existing single-flux-quantum (SFQ) superconducting circuits. Using a multi-tip scanning tunnelling microscope (STM) we investigated the microscopic behaviour of the CCM device during operation. By analysing the evolution of the polaronic configurations (Fig. 1) while incrementally increasing electrical current excitation, we observed non-trivial topological defects in the form of dislocations, which are responsible for the non-volatility of the CCM device. The manuscript was submitted to Nature Electronics.

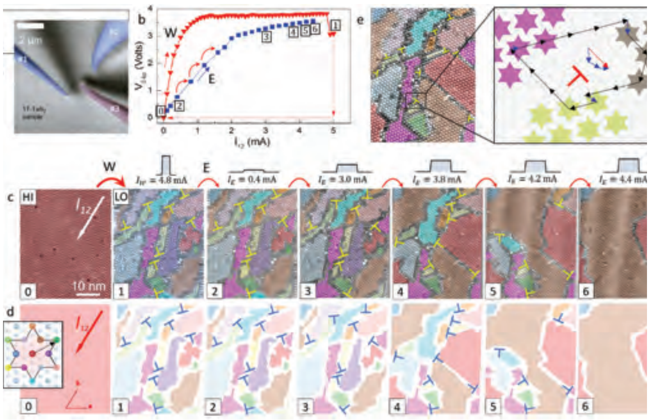

Figure 1: Figure showing the experiment in the STM. a) SEM image of the STM tips and the 1T-TaS_2 sample in the background. b) Voltage-current characteristics for the Write (W) and Erase process. c, d) Evolution of the charge configuration during the CCM device's operation. e) Burger's vector construction.

Ultrafast studies of non-equilibrium quantum matter.

Metastable, self-organized electronic states in quantum materials are of fundamental importance, displaying new, emergent, dynamical properties that can be used in new generations of sensors and memory devices. Such states are typically formed through a phase transition under non-equilibrium conditions. By using time-resolved optical techniques and femtosecond-pulse-excited scanning tunnelling microscopy, the evolution of the metastable states in the quasi-two-dimensional dichalcogenide 1*T*-TaS_2 are mapped out on a temporal phase diagram using photon density and temperature as the control parameters on timescales ranging from 10^{-13} to 10^3 s.

The introduction of a time-domain axis in the phase diagram enables us to follow the time evolution of processes created through different phase-transition mechanisms that lead to metastable emergent states on different

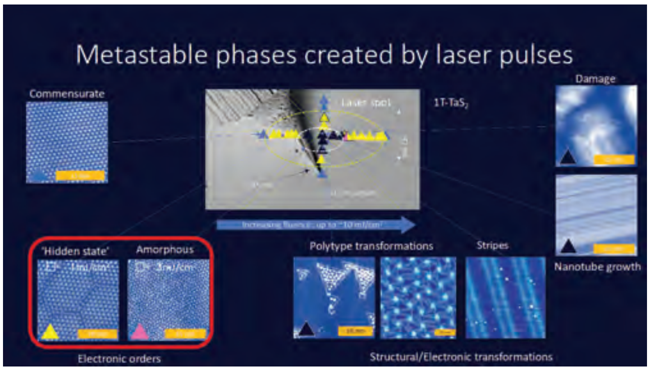

Figure 2: Metastable phases created by femtosecond laser pulses in a transition-metal dichalcogenide material. The material is excited inside an STM chamber (Omicron LP 4-probe). The excited area is shown in the SEM image (middle). Different topological phases are excited at different laser intensities.

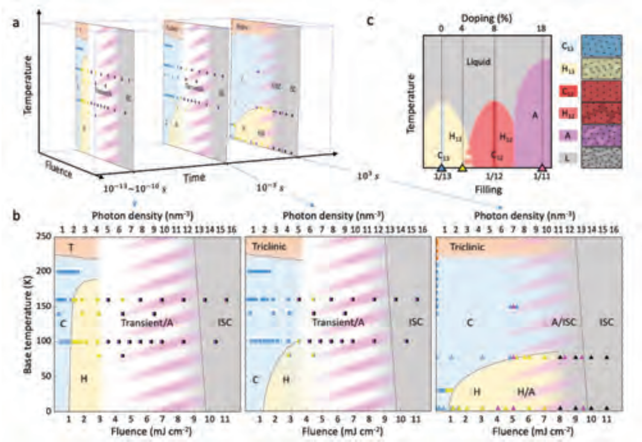

Figure 3: The time-domain phase diagram. a) Schematic timeline of the phase-diagram evolution b) Detailed phase diagrams on the three timescales, as indicated. Triangles represent the scanning tunnelling microscopy (STM) data and squares represent the transient reflectivity data. c) The equilibrium phase diagram obtained from simulations.

Phase diagrams are usually considered to describe equilibrium phases. For the first time we now present a non-equilibrium phase diagram, in which the Qtime evolution of different phases of a quantum material are presented on timescales ranging from femtoseconds to minutes. The work can be found in a paper published in Nature Communications.

timescales, thus opening the way to understanding the complex ordering processes in metastable materials. The experimental phase diagram is supported by theoretical calculations (see Figure). A paper in **Nature Communications** describes the results (to appear in 2021).

Ultrafast transient reflectivity across the unusual three-dimensional Peierls-like insulator-metal (IM) transition in $CuIr_2S_4$ was measured as a function of temperature and excitation fluence. The low-temperature insulating phase's transient response is dominated by broken-symmetry-induced coherent lattice oscillations that abruptly vanish at the IM transition. The coherent mode spectra are consistent with Raman spectra reported in the literature. The origin of the broken-symmetry-induced modes and the photo-excited carrier recombination pathway through in-gap defect states were also briefly discussed. The results were published in **Phys. Rev. B 101, 165134 (2020).**

The Low-T symmetry-broken insulating state in $CuIr_2S_4$ is also interesting due to the existence of a metastable, irradiation-induced, disordered, weakly conducting state. We continued the study of intense femtosecond optical pulse irradiation effects by means of the all-optical, ultra-fast, multi-pulse, time-resolved spectroscopy. We showed that the structural coherence of the Low-T broken-symmetry state is strongly suppressed on a sub-picosecond timescale above a threshold excitation fluence resulting in a structurally inhomogeneous transient state that persists for several-tens of picoseconds before reverting to the Low-*T*, disordered, weakly conducting state. The electronic order shows a transient gap filling at a significantly lower fluence threshold. 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 ultra-fast 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. The manuscript was submitted to **New Journal of Physics**.

In collaboration with the department F6 we investigated the incorporation of a Cu dopant into a host structure of ferroelectric $Sn_2P_2S_6$ by means of coherent phonon spectroscopy. The integration of dopant atoms into the bulk of an already-grown crystal could be easily tuned up to 0.5 at%, affecting the structural, optical, vibrational, electrical, and ferroelectric properties. Thermally diffused copper atoms in $Sn_2P_2S_6$ bulk induce a multi-axial expansion of the $Sn_2P_2S_6$ unit cell by 2–3.4%. The energy reduction between the indirect and direct optical transitions was observed, combined by small hardening for acoustic and soft optical vibrational modes originating in the partial substitution of Sn by Cu in the $Sn_2P_2S_6$ crystal lattice. The results were published as a part of a broader study in **J. Mater. Chem. C 8, 9975 (2020).**

Theoretical studies on the nanoscale

Applying the GGA+U approach, the structural, electronic and magnetic properties of $LaMnO_3/BaTiO_3$ heterostructure were investigated. Special attention was concentrated on the analysis of the heterostructure with ferroelectric polarization in the $BaTiO_3$ film oriented perpendicular to the $LaMnO_3$ substrate. Atomic and spin-resolved density of states were calculated for the $LaMnO_3/BaTiO_3$ heterostructure with different numbers of $BaTiO_3$. It was found that the $LaMnO_3/BaTiO_3$ heterostructure becomes conducting with a significant spin polarization, indicating that the interface becomes ferromagnetically ordered. The proposed concept of a ferroelectrically controlled interface ferromagnetism offers the possibility to design novel electronic devices. (**Mater. Res. Express, 7, 055020 (2020).**)

A short overview of theoretical models for the description of the relaxation processes in metals excited by a short laser pulse is presented. The main effort is given to a description of different processes that are taking place after the absorption of the laser pulse. The widely used, two-temperature model is discussed and the conditions of applicability for this model are identified. Various approaches to solving the Boltzmann kinetic equations are discussed. It is identified that in the case of a low excitation limit the relaxation is determined by the emission of phonons by photo-excited electrons. The possibility to obtain the value of the electron phonon coupling constant from experiments is discussed. (**Low Temp. Phys. 46, 414 (2020)**.)

We addressed the problem of microscopic processes leading to macroscopic quantum tunnelling (MQT) in a quantum system. We investigated quantum electron reconfiguration dynamics in two matching embodiments: domain relaxation in a prototypical two-dimensionally electronically ordered solid-state quantum material, and a matching simulation setup in a quantum computer. The understanding of quantum many-body reconfigurations by MQT advances our understanding in diverse condensed quantum matter. A manuscript has been submitted to **Science**, and is currently under review.

We studied 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. A comparison of the 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. A manuscript has been submitted to **Nature Communications**, and is currently under review.

Mirrored domains are experimentally very rarely found in a single crystal and thus very rarely investigated. However, it was recently shown in STM studies (Figure 1) that applying an ultrafast laser pulse to a thin flake of 1T-TaS_2 we can switch between the two mirrored superlattice orientations. It is not clear whether this is an interlayer or an intralayer effect, and how the domains order and interact at the microscopic level. We employed the theoretical model we developed for 1T-TaS_2 in order to investigate the origin of the various domain structures we found. A manuscript is currently in preparation.

Apart from the work mentioned above, a number of papers appeared as a result of collaborations, which are listed in the bibliography.

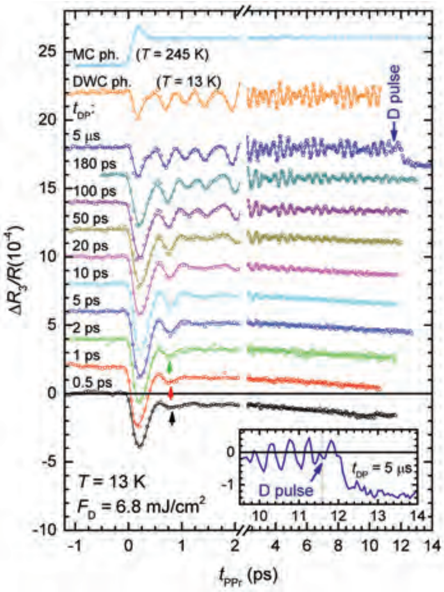

Figure 4: Multi-pulse transient reflectivity as a function of the delay between the driving and pump pulses, tDP . The arrow at the tDP =5-µs scan indicates the arrival of the subsequent driving pulse. The two top-most traces, shown for comparison, correspond to the thermal equilibrium metallic- and low-temperature-phase transient reflectivity.

Nanomaterials

We discovered an optimization of carbon nanofibre (CNF) growth on molybdenum carbide nanowires (MoCNW) by the direct carburization of $Mo_6S_2I_8$ nanowire bundles in a mixture of ethane, argon and hydrogen at 700 °C. Typical CNFs obtained with this method are several hundreds of nanometres long with a diameter of 10–20 nm. The fast release of iodine and sulphur atoms during the nanowire's hydrogenation controlled by heating rate, results in the formation of smaller particles with an average diameter of around 10 nm. When ethane is included in the reaction, carbon dissolves and diffuses through the molybdenum grains until it is deposited on the other side in the form of graphite. Carbon deposition and nanofibre growth continue and the nanoparticles, which serve as catalyst seeds for growing carbon nanofibres, are lifted away from the surface.

We show that nanofibre growth does not depend on the initial morphology of the nanowires: nanofibres grow on individual bundles of MoCNW, on dense networks of nanowires deposited on silicon substrate, and on free-standing nanowire foils. We find that carbon nanofibres remain firmly attached to the nanowires even if they are modified into Mo_2C and further into MoS_2 nanowires at 800 °C. The method thus enables the production of a novel, hybrid material composed of MoS_2 nanowires densely covered with carbon nanofibres. This proves that the applied approach is not limited to carbon nanofibre growth and the fabrication of molybdenum carbide-based hybrid materials, but enables the fabrication of other molybdenum-based hybrid materials as well. We have additionally shown that the obtained CNFs can easily be self-decorated with platinum nanoparticles with diameters of several nanometres, directly from a water solution at room temperature without reducing agents. Such an efficient synthesis and decoration process yields hybrid platinum/CNF/molybdenum-based NW materials, which are a promising material for a wide range of possible future applications, including sensitive sensorics and improved catalysis. The work was published in **R Soc Open Sci.**

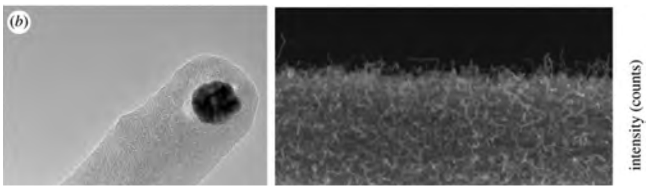

Figure 5: TEM image of carbon nanofibers grown on molybdenum carbide nanowires:
(a) nanowire covered with fibres; (b) a single carbon nanofibre with a Mo2C nanoparticle. SEM image of hybrid material.

Soft Matter

We continued to investigate tuneable optical diffraction structures based on liquid crystals that are introduced into laser written polymeric scaffolds (our patent WO2015139353 (A1)). A theoretical work on magnetically tuneable optical diffraction gratings fabricated by introducing a ferromagnetic liquid crystal into such scaffolds was reported in **Polymers**, **12**, 2355 (2020).

In cooperation with Nankai University in China we investigated the process of random lasing in dye-doped cholesteric liquid crystals (CLCs). The concentration of the chiral agent was changed to tune the bandgap, and disordered CLC microdomains were achieved by fast quenching of the mixture from the isotropic to the cholesteric phase. The results showed that the threshold for random lasing sharply decreases if the CLC selective reflection band overlaps with the fluorescence peak of the dye molecules and if, at the same time, the band edge coincides with the excitation wavelength. The work was published in **Photonics research**, 8, 642 (2020). We also completed common investigations of intercellular communication over the intercellular bridge that is formed between the two daughter cells at the end stage of the cytokinesis process. The results of this work were published in **Biophysical journal, 5**, 1196 (2020). Besides this, in 2020 our research collaboration was extended to the topic of multifunctional metamaterials based on graphene. The results of this work were published in **Optics express**, **28**, 24772 (2020). The main idea of this work was also patented in the Chinese **patent** (CN 107244669 A).

In cooperation with the group of J. Plavec from the National Institute of Chemistry (KI) we investigated the mechanisms of G-quadruplex formation in the DNA sequences GCn and GCnCG, where n=G2AG4AG2 in the presence of Na+ ions. We found that G-quadruplexes exhibit unique combinations of structural elements, among which are two G-quartets, A(GGGG)A hexad and a GCGC-quartet. This knowledge will be used as a base for designing DNA sequences for nanotechnological applications that require specific folding and multimerization properties. The results were published in **Nucleic Acids Research**, 48, 2749 (2020).

We continued with studies and the development of suspensions of magnetic nanoplatelets in isotropic solvents, which at high enough concentrations exhibit ferromagnetic order. In collaboration with researchers from the University of Vienna, we focused on investigations of the influence of polydispersity on the structural properties of the isotropic phase of magnetic nanoplatelets using a combination of molecular dynamics simulations and experimental SAXS studies. We showed how the polydispersity can lead to the reduction of the orientational and spatial correlations in the absence of an applied field, while simultaneously facilitating the field-induced transition into a nematic-like phase (**Journal of Molecular Liquids 312**, 113293 (2020)). In collaboration with researchers from Department for Materials Synthesis (K8), we studied the formation of Fe(III)-phosphonate porous coatings on barium hexaferrite (BHF) nanoplatelets. The so-obtained porous nanomagnets are highly responsive to a very weak magnetic field (of the order of the Earth's magnetic field) at room temperature, which is a major advantage over the classic mesoporous nanomaterials and metal–organo-phosphonic frameworks with only a weak magnetic response at a few kelvins. The combination of porosity with the intrinsic magnetocrystalline anisotropy of BHF can be exploited, for example, as sorbents for heavy metals from contaminated water (**ACS Omega 5** (23), 14086-14095 (2020)).

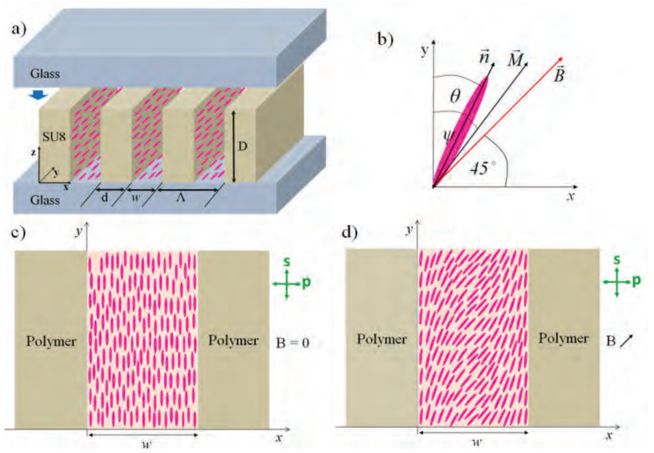

Figure 6: Magnetically tenable optical diffraction grating. a) Schematic drawing of the periodic assembly of ferromagnetic liquid-crystal (LC) channels separated by polymeric ribbons. Stripes indicate the polymer ribbons and pink ellipsoids indicate the LC molecules. b) Local orientation of the nematic director n and of the magnetization M under the influence of the external magnetic field B. (c) Schematic drawing of the homogeneous alignment of the LC medium between two polymer ribbons at B = 0. Alignment along the y-axis is induced by the surface relief structure present on the sidewalls of the ribbons. (d) Schematic drawing of the in-plane reorientation of the LC molecules induced by an external magnetic field tilted at 45° with respect to the y-axis. [D. Bošnjaković et al., Polymers 2020, 12, 2355]

In collaboration with researchers from the University of York and the University of Leeds, UK, we continued investigations of recently designed ferroelectric splay nematic phase. We showed that the transition between the uniaxial and the splay nematic phase is a ferroelectric-ferroelastic phase transition, in which flexoelectric coupling causes the simultaneous occurrence of diverging behaviour of electric susceptibility and of instability towards splay deformation. This study was published in ***Phys. Rev. Lett.*** **124**, 037801(2020). It was chosen by the editors as an Editors' Suggestion, and highlighted in the journal Physics Today. We also proposed a unified phenomenological Q-tensor model of twist-bend (N_{TB}) and splay nematic (N_S) phases. We modelled both phases with a single Q-tensor free energy including a term that breaks the degeneracy between the splay and bend elastic constant, and a flexoelectric term coupling the divergence of the Q-tensor with polarization. The N_{TB} or N_S phase is obtained by a change of sign of one elastic parameter (**Phys. Rev. E 101**, 022704 (2020)).

In collaboration with researchers from the Department of Physical and Organic Chemistry (K3), we studied the polymerization dynamics of an acrylate-based, hybrid, sol-gel coating for the corrosion protection of AA7075-T6 for aircraft applications. The goal of the study was to identify the impact of copolymerization time on the structure and morphology of a hybrid material composed of acrylate monomers and a siloxane network. The results indicated that the proposed optimised coating can function as a pre-treatment for the long-lasting corrosion protection of AA7075-T6 (**Polymers 12**, 948 (2020)).

Biomedical optics

We have continued with the development of innovative optical techniques for biomedical applications. By combining pulsed photo-thermal radiometry (PPTR; time-resolved measurements of laser-induced mid-infrared emission) and diffuse reflectance spectroscopy (DRS) with a dedicated numerical model of light transport in strongly scattering biological tissues, we have developed a unique approach for non-invasive characterization of human skin *in vivo*. This approach enables a non-invasive assessment of several physiologically relevant parameters (e.g., the contents and oxygen saturation levels of blood in different skin layers), in parallel with structural and scattering properties of the epidermis and dermis.

However, the involved iterative inverse analysis is computationally very expensive. In order to overcome this drawback, we have constructed a predictive model based on machine-learning technology. Its application significantly shortens the computation times, while at the same time improving the robustness and accuracy of the results. (Collaboration with Department of Knowledge Technologies, IJS). **Biomed. Opt. Express 11, 1679-1696, 2020**

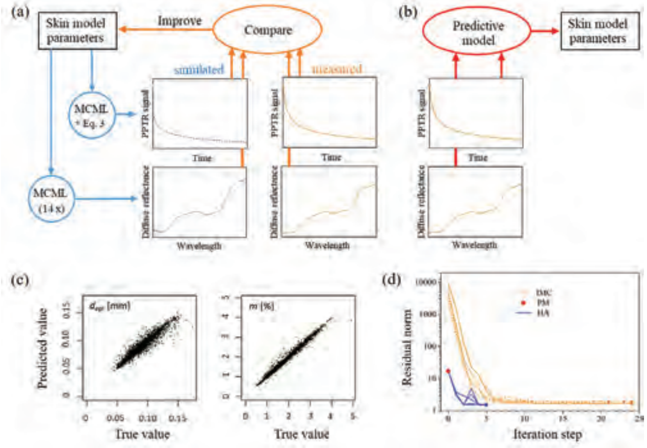

Figure 7: Schematic presentation of the assessment of 13 properties of human skin from experimental data using: a) iterative multi-dimensional optimization, and b) the predictive model (PM). c) Results of cross-validation testing for two skin-model parameters (the epidermal thickness and melanin content). d) Initializing the iterative optimization procedure (IMC) with the PM result reduces the computation time and improves the results (blue lines).

Supporting our unique methodology for non-invasive characterization of human skin in vivo with machine-learning technology led to significantly reduced computation times, improved accuracy, and lower variance of the results.

The described methodology was further augmented and applied to the characterization of laser tattoo removal and longitudinal monitoring of traumatic bruises in human volunteers. Such methodology and improved understanding of the underlying processes could enable the optimization of the tattoo removal treatment and the development of a more accurate bruise-aging methodology for forensic investigations. (**Proc. SPIE vol. 11211, 112110X, 2020; Sensors 21, 302, 2020**)

Microfluidics

Microfluidic research is conducted in close collaboration with the Laboratory for Experimental Soft Matter at the Faculty of Mathematics and Physics, University of Ljubljana. Based on a successful analysis of fluid flow in microfluidic side chambers, we have developed a new type of microfluidic flow sensor. The velocity of the liquid in the microfluidic sample is measured indirectly, by observing dynamics of a non-miscible liquid in side chambers. By monitoring the movement of tracer particles in the side channels, we determined the characteristic flow parameters and showed a linear relationship with the fluid velocity over a wide range of measured velocities. The description of the experimental method was published in **IEEE Sensors Journal**.

A second area of research was devoted to the manipulation of nanoparticles in liquids. We have experimentally demonstrated the transport of particles with optically induced, temporally varying temperature gradients. By real-time object tracking and control of the position of the heating laser focus, we were able to precisely employ thermophoretic drift to oppose the random diffusive motion, creating a trap for nanoparticles. Multiple traps can be dynamically created and relocated, which we demonstrated by the controlled, independent manipulation of two nanoparticles. A numerical model predicted the observed effect and supported the experimental results. The findings of the research were published in **Beilstein Journal of Nanotechnology**.

We have developed a non-invasive method for measuring the fluid flow in microfluidic channels, based on observations of secondary induced currents in side chambers.

The third broader area of microfluidic research involves observations of particle dynamics in liquids. In collaboration with industrial partners, we are developing experimental methods for studying the motion of nanoparticles in a fluid, the aggregation of particles at surfaces and particle deposition on boundaries. The various experimental methods we have developed offer complementary results that allow for a rapid and simple quantitative sample analysis, which is particularly interesting for industrial use. In addition, we investigate the motion of magnetic particles in a fluid flow. Particle motion results in the appearance of a magnetic field, which can be measured, and the occurrence of birefringence, which can be observed. Research of the magnetic particle dynamics is still ongoing.

Some outstanding publications in the past year

1. Čopič, Martin, Mertelj, Alenka. Q-tensor model of twist-bend and splay nematic phases. Physical review. E, ISSN 2470-0045, 2020, vol. 101, no. 2, str. 022704-1-022704-6, doi: 10.1103/PhysRevE.101.022704. [COBISS.SIID 33233191]

2. Sebastián Ugarteche, Nerea, Cmok, Luka, Mandle, Richard J., Fuente, Maria Rosario De La, Drevenšek Olenik, Irena, Čopič, Martin, Mertelj, Alenka. Ferroelectric-ferroelastic phase transition in anematic liquid crystal. **Physical review letters**, ISSN 0031-9007. [Print ed.], 2020, vol. 124, no. 3, str. 037801-1-037801-6, doi: 10.1103/PhysRevLett.124.037801. [COBISS.SI-ID 33088039]
3. Konrad Gillmeister, Denis Golež, Chiang Cheng-Tien, Nikolaj Bittner, Yaroslav Pavlyukh, Jamal Berakdar, Philipp Werner, Wolf Widdra, "Ultrafast coupled charge and spin dynamics instrongly correlated NiO", Nature communications, vol. 11, str. 4095-1-4095-9, 2020, doi: 10.1038/s41467-020-17925-8. [COBISS.SI-ID 46013187]
4. Denis Golež, Zhiyuan Sun, Yuta Murakami, Antoine Georges, Andrew J. Millis, "Nonlinear spectroscopy of collective modes in an excitonic insulator", Phys. rev. lett., vol. 125, no. 25, str. 257601-1-257601-6, 2020, doi: 10.1103/PhysRevLett.125.257601. [COBISS.SI-ID 46028803]
5. Mimoza Naseska, Petra Šutar, Damjan Vengust, S. Tsuchiya, Miran Čeh, Dragan Mihailović, Tomaž Mertelj, "Orbitally driven insulator-metal transition in CuIr2S4CuIr2S4 etemperature-dependent transient reflectivity study", Physical review. B, vol. 101, no. 16, str. 165134-1-165134-6, 2020, doi: 10.1103/PhysRevB.101.165134. [COBISS.SI-ID 27075075]
6. Steven D. Conradson, Venera Nasretdinova, et al., "Nonadiabatic coupling of the dynamical structure to the superconductivity in YSr2Cur2.75Mo0.25O7.54YSr2Cur2.75Mo0.25O7.54 and Sr2CurO3.3Sr2CurO3.3", Proc. Natl. Acad. Sci. U. S. A., 8 str., [in press] 2020, doi: 10.1073/pnas.2018336117. [COBISS.SI-ID 43427587]
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8. Verdel, Nina, Tanevski, Jovan, Džeroski, Sašo, Majaron, Boris. Predictive model for quantitative analysis of human skin using photothermal radiometry and diffuse reflectance spectroscopy. *Biomedical optics express*, ISSN 2156-7085, 2020, vol. 11, no. 3, str.1679-1696, doi: 10.1364/BOE.384982. [COBISS.SI-ID 33232423]

Awards and Appointments

1. Dr. Igor Vaskivskyi: Winner of the Director's Fund for the Laboratory for 4D Resonance Magnetic Spectroscopy project , 20 April2020
2. Asst. Prof. Alenka Mertelj: Mid-Career Research Excellence Award, ILCS (The International Liquid Crystal Society) for discovery of both magnetic and electric polar order in nematic phase and new spatially modulated splay nematic phase that has macroscopic electric polarization, 2020
3. Prof. dr. Dragan Mihailović, Damjan Svetin, Anže Mraz, Rok Venturini: Gold medal at the 18th International Innovation Exhibition ARCA 2020 for poster Innovative superconductor-based memory device and method for its operation, using a switchable resistive element suitable for superconducting computing – compatible with superconducting flex-quantum electronics, Zagreb, Croatia
4. Prof. dr. Dragan Mihailović, Damjan Svetin, Anže Mraz, Rok Venturini: Silver medal at the 1st virtual fair of innovation and entrepreneurship "Sarajevo 2020" for Memory device and method for its operation, Startup studio Fondacije Mozaik in Sarajevo Business Forum (SBF), Bosna in Hercegovina, 24. 11. 2020

Organization of conferences, congresses and meetings

1. Nonequilibrium Dynamics and Ergodicity of Complex Quantum Systems, Krvavec, Slovenia, 14–17 December 2020 (virtually)

Patents granted

1. Marko Kazič, Matjaž Lukač, Laser treatment head and laser system, EP2957323 (B1), European Patent Office, 23. 12. 2020.
2. Xinzheng Zhang, Jingjun Xu, Bin Shi, Xiaodan Xu, Yang Liu, Mengxin Ren, Wei Cai, Qiang Wu, Irena Drevenšek Olenik, Processing method and processing system for laser-induced graphene micronano structure, CN107244669 (B), State Intellectual Property Office of the P.R.C., 25. 12. 2020.

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. H2020 - MAGNELIQ; A Magneto-Electric Liquid - Better Sensing
   Asst. Prof. Alenka Mertelj
   European Commission
6. Liquid Crystalline Properties of Guanosine-Rich DNA and RNA Oligonucleotides
   Prof. Irena Drevenšek Olenik
   Slovenian Research Agency
7. Microstructuring of Liquid Crystals and Light Wave Manipulation by Photorefractive Materials
   Prof. Irena Drevenšek Olenik
   Slovenian Research Agency
8. Studies of Structure and Dynamics of Liquid Magnets by SAXS and SANS
   Asst. Prof. Alenka Mertelj
   Slovenian Research Agency
9. Tunable Optical Diffractive Structures from Liquid Crystalline Materials
   Prof. Irena Drevenšek Olenik
   Slovenian Research Agency
10. Novel Liquid Crystalline Materials for Application in Diffractive Optical Elements
    Prof. Irena Drevenšek Olenik
    Slovenian Research Agency
11. 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. Femtosecond time-resolved scanning tunneling electron microscopy of complex materials
   Prof. Dragan Dragoljub Mihailović
2. Electrically tunable ferromagnetic liquids
   Asst. Prof. Alenka Mertelj
3. Probing spin states near the surface of quantum spin materials
   Petra Šutar
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. Development of gradual optical shutter – OPTIGRAD
   Dr. Luka Cmok
   Ministry of Education, Science and Sport
10. Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF)
    Prof. Dragan Dragoljub Mihailović
    Ministry of Economic Development and Technology
11. CMEM: Ultrafast all-electronic charge density wave memory for next generation computing
    Dr. Igor Vaskivskyi
    Ministry of Education, Science and Sport
12. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
    Prof. Dragan Dragoljub Mihailović
    Slovenian Research Agency

VISITORS FROM ABROAD

1. Dr Rinat Mamin, Zavoisky Physical-Technical Inst. of FIC KazanSC, Kazan, Russia, 16 January to 1 February 2020
2. Héloïse Orihuel, Marseille University, Marseille, France, 3 February to 1 August 2020
3. Prof. Toda Yasunori, Hokkaido University, Sapporo, Japan, 20 February to 4 March 2020
4. Dejan Bošnjaković, Faculty of Electrical Engineering, Computer Science and Information Technology Osijek, Croatia, 9–10 March2020
5. Dipl. ing. Inna Belyaeva, Faculty of Electrical Engineering and Information Technology, OTH Regensburg, Germany, 24 July to 3 August 2020
6. Dominik Brandl, Faculty of Electrical Engineering and Information Technology, OTH Regensburg, Germany, 2 August to 28 September 2020
7. Prof. dr. Mikhail Chamonine, Faculty of Electrical Engineering and Information Technology, OTH Regensburg, Germany, 15–22 September 2020

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18. *Dr. Iaroslav Gerasimenko, left 01.03.20*
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25. Andrej Kranjec, B. Sc.
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38. Martina Knavs, B. Sc.

Note:
* part-time JSI member

BIBLIOGRAPHY

ORIGINAL ARTICLE

1. Darja Lisjak, Patricija Hribar, Alenka Mertelj, Andraž Mavrič, Matjaž Valant, Janez Kovač, Hermina Hudelja, Andraž Kocjan, Darko Makovec, "Formation of Fe(III)-phosphonate coatings on barium hexaferrite nanoplatelets for porous nanomagnets", *ACS omega*, 2020, **5**, 23, 14086-14095.
2. Urška Trstenjak, Damjan Vengust, Zoran Samardžija, Aleksander Matavž, Vid Bobnar, Danilo Suvorov, Matjaž Spreitzer, "Stabilization of the perovskite phase in PMN-PT epitaxial thin films via increased interface roughness", *Applied Surface Science*, 2020, **513**, 145787.
3. Vasyl Shvalya, Gregor Filipič, Damjan Vengust, Janez Zavašnik, Martina Modic, Ibrahim Abdulhalin, Uroš Cvelbar, "Reusable Au/Pd-coated chestnut-like copper oxide SERS substrates with ultra-fast self-recovery", *Applied Surface Science*, 2020, **517**, 146205.
4. Jošt Stergar, Natan Osterman, "Thermophoretic tweezers for single nanoparticle manipulation", *Beilstein journal of nanotechnology*, 2020, **11**, 1126-1133.
5. Nina Verdel, Jovan Tanevski, Sašo Džeroski, Boris Majaron, "Predictive model for quantitative analysis of human skin using photothermal radiometry and diffuse reflectance spectroscopy", *Biomedical optics express*, 2020, **11**, 3, 1679-1696.
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22. Daša Pavc, Baifan Wang, Lea Spindler, Irena Drevenšek Olenik, Janez Plavec, Primož Šket, "GC ends control topology of DNA G-quadruplexes and their cation-dependent assembly", *Nucleic acids research*, 2020, **48**, 5, 2749-2761.
23. Yang Liu *et al.* (12 authors), "Multifunctional and tunable trigate graphene metamaterial with "Lakes of Wada" topology", *Optics express*, 2020, **28**, 17, 24772-24788.
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25. Shaohua Gao, Jiayi Wang, Wenhua Li, Xuanyi Yu, Xinzheng Zhang, Xiao Song, Andrey Iljin, Irena Drevenšek Olenik, Romano Anton Rupp, Jingjun Xu, "Low threshold random lasing in dye-doped and strongly disordered chiral liquid crystals", *Photonics research*, 2020, **8**, 5, 642-647.
26. Nerea Sebastián Ugarteche, Luka Cmok, Richard J. Mandle, Maria Rosario de la Fuente, Irena Drevenšek Olenik, Martin Čopič, Alenka Mertelj, "Ferroelectric-ferroelastic phase transition in a nematic liquid crystal", *Physical review letters*, 2020, **124**, 3, 037801.
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charge transport in organic crystals", *Physical review. X*, 2020, **10**, 2, 021062.
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2. Ana Marin, Nina Verdel, Boris Majaron, "Hemodynamics in traumatic bruises assessed by diffuse reflectance spectroscopy and photothermal radiometry", In: *SPIE BIOS, 1-6 February 2020, San Francisco, California, United States*, Proceedings, Photonics in dermatology and plastic surgery 2020, (Proceedings of SPIE **11211**), SPIE, 2020, 112110z.
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1. Matjaž Ličen, *Photoregulation of molecular assembly in thin surface films:* doctoral dissertation, Ljubljana, 2020 (mentor Irena Drevenšek-Olenik).
2. Nina Verdel, *Characterization of human skin by combined photothermal radiometry and diffuse reflectance spectroscopy:* doctoral dissertation, Ljubljana, 2020 (mentor Boris Majaron; co-mentor Matjaž Lukač).

DEPARTMENT OF REACTOR PHYSICS F-8

Head:
Prof. Luka Snoj

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***

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

The main objective of the project entitled *Stability of nuclear reactors in load follow mode of operation,* which started in 2020, is to 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 to the plant operator for optimizing the plant's operation. In 2020, communications with all partners, including the industry partners, were established. Additionally, research activities on all work packages started and are proceeding according to the envisioned time schedule. The first research results are expected to be produced 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 the corresponding covariance data in a rigorous manner that is from first principles, by employing state-of-the-art atomistic simulations, which rely on the density functional theory in combination with lattice or molecular dynamics calculations. As part of the project's activities regarding atomistic simulations for the needs of producing thermal scattering data have begun. Additionally, communication channels have been established with the North Carolina State University, whose experts will contribute the know-how which will result in the successful start of the project. The work on the project is proceeding according to the time schedule envisioned in the project proposal. The first research results are expected to be produced in 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, also 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.

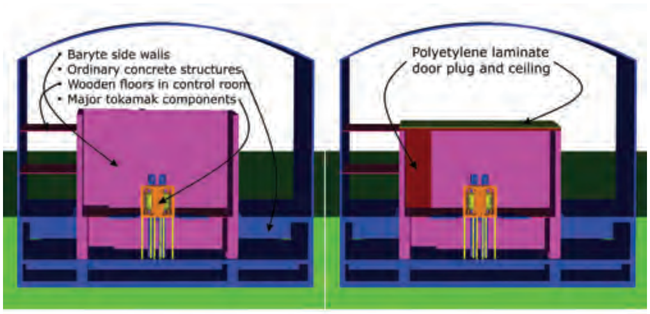

Figure 1: TCV tokamak basic and updated computational model.

The primary objective of the European TOURR project that started in 2020 is to develop a strategy for Research Reactors in Europe and prepare the ground for its implementation. This strategic goal can be divided into specific objectives: Assessment of the current status of European RR fleet, including plans for upgrade; evaluation of urgent EU needs; developing tools for optimal use of RR fleet and rising awareness among decision makers on the (future) role of RRs. 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.

The aim of the project entitled *Determination and shielding upgrade of the TCV tokamak* was to estimate the reduction in neutron dose rates within the "Tokamak à configuration variable" or "Variable configuration tokamak" (TCV) building after adding a ceiling and installing a shielded door at the TCV hall entrance. The analysis was subdivided into three tasks. This included a comparison of several different shielding materials at different thicknesses in the first task and the effect of existing gaps in the concrete walls in the second task. The material shielding task showed Shieldwerx SWX201 borated polyethylene was the best-performing material closely followed by a laminate polyethylene/borated polyethylene material. The gap analysis showed that total dose from the gaps in the concrete walls was insignificant. In the third and final task an upgraded MCNP model (reference model) was used for dose-field calculations and dose-rate calculations at specific locations around the TCV machine. The project was a success and the provided data will be used as an engineering basis for actual shielding designs. The project also served to establish connections with the TCV team for future research activities.

Researchers of the Reactor Physics Department provided technical support for the safe and economic operation of the Krško Nuclear Power Plant (NPP) in 2020. We performed initial nuclear design calculations for the cycle 32 and provided support for the determination of the fresh fuel characteristics. Our independent expert evaluation has confirmed that the 5 % increase with respect to the equilibrium 18-month cycle burnup considered in the NPP Krško safety analysis of radiological consequences of design basis accidents will not result in a dose increase that is "more than minimal", as defined by the guidance in NEI 96-07. In the framework of the applied project financed by the Slovenian Research Agency (co-financed by the NPP Krško) "Development of Computational Tools for the Determination of the Neutron Field in the Containment of a Pressurized Water Reactor" calibration and verification process has been performed at HZP and HFP conditions. Several calculations have been made to analyse the neutron detector's response.

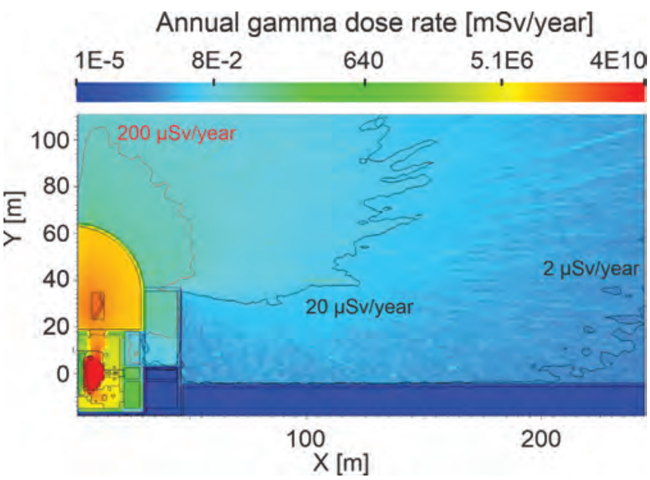

Figure 2: Annual gamma dose rates around the fusion reactor DEMO during the maintenance of the breeding blanket.

In 2020 we have been working on the project "Support for implementation and calculations in the SFDS project", whose aim is to support NEK power plant in design and implementation of the dry storage repository for spent fuel. According to an agreement with NEK, we have been conducting studies and improvements needed to increase the accuracy of the spent fuel source term and help reduce uncertainty in future core design calculations for NEK. We have generated new ISOLIB libraries based on nuclear data libraries ENDF/B-VIII, JEFF-3.3 in JEFF-4T and compared the isotopic compositions from the generated libraries with previous calculations. We have developed multiple updates to the CORD-2 source code, which will simplify its use with modern compilers, such as new versions of gfortran.

In the framework of the internation 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), their goal is the development of pixelized detectors that will enable the simultaneous detection of thermal and fast neutrons, charged particles and X-ray 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.

In 2020 we completed a project for the French Institute IRSN (Institut de Radioprotection et de Sûreté Nucléaire) as part of a consortium with IDOM. In the project entitled *Activation Calculations of Metallic Nozzles of Fuel Assemblies*, we analysed the inventory of radioisotopes, primarily ^{60}Co, in the nozzles of fuel elements in different fuel-cycle scenarios. Time-dependent calculations were performed with the MCNP transport code, whereby a precise model of the fuel element with the upper and lower nozzle was made.

Within the given project, we checked the burn-up calculations for the case of a light-water fuel element with the SCALE 6.2 package. In three phases, for the fuel element containing UO2 or MOX fuel, we performed calculations with the ORIGEN module, then with the 2D TRITON, and with the 3-D KENO model and compared the calculations with the reference calculations provided by IRSN.

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 2020 we carried out two experimental testing campaigns.

In 2020 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 safe disposal of low and intermediate level radioactive waste. We performed a study on the radiolysis of super-plastificators through gamma irradiations at the JSI TRIGA reactor. In WP8 we have 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 the sensitivity and uncertainty analyses with the use of different codes and models.

In 2020 we continued our collaboration efforts in the framework of the European project ENEEP - European Nuclear Experimental Educational Platform. The aim of the project is the establishment of 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 2020 we collaborated mostly in WP3 of the project, with the aim of collecting information on experimental facilities and equipment, educational activities and potential users and the performance of a SWOT analysis. We have initiated work on WP4, which we are coordinating, with the objective to perform the activities required for the establishment of the platform itself.

In collaboration with colleagues from CEA Cadarache we continued with research on the feasibility of using 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 the capability of online neutron flux measurements in challenging conditions, as the neutron flux level changes by 6–7 orders of magnitude in a few ms. In 2020 we performed a series of test measurements of Cherenkov light intensity in reactor pulse mode as an alternative and physically independent method of reactor power measurement, and activation measurements. An experimental campaign is scheduled in 2021 in which simultaneous measurements of the signals of miniature fission chambers, Cherenkov light intensity and activation measurements will be performed.

In 2020 in collaboration with colleagues from CEA Cadarache activities we initiated 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 the performance of 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, thermo-luminescent detectors), and the comparison of the experimental data with the results of simulations performed using the Monte Carlo method. The experimental campaign is scheduled in mid-2021.

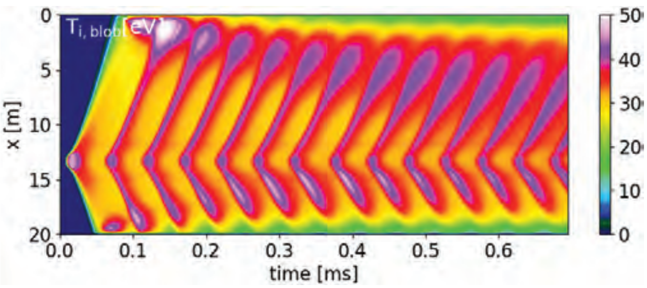

Figure 3: The evolution of blob-filament temperature (in eV) from a PIC-MCC simulation of train of blobs-filaments entering the scrape-off layer region of a tokamak. x=0 m is the inner divertor, x= 13 m is the blob source and x=20 m is the outer divertor. The slope of the colour trace represents the ion sound speed. The temperature drop at the divertors is due to charge-exchange processes with neutrals that build up due to ion recycling.

In collaboration with CEA Cadarache, activities regarding planning of 241Am thermal neutron capture cross-section measurements were continued. A measurement of 242Am/242Cm activation was performed in the central irradiation channel of the JSI TRIGA reactor using low-activity 241Am samples, produced at the JSI. Optimal initial activities of 241Am samples for irradiation in other irradiation channels of the JSI TRIGA reactor were calculated, and the experimental campaign at TRIGA is planned for 2021.

In collaboration with CEA Cadarache we analysed benchmark experiments, which were performed in the United Kingdom at the NESTOR/Winfrith reactor within the ASPIS experimental setup. Besides the APSIS Iron88 experiment, which is already part of SINBAD, we contributed to the analysis of other experiments that are not part of SINBAD yet. At the JSI we performed a simulation with the MCNP Monte Carlo code using several nuclear data libraries including ENDF/B-VIII.0, /B-VII, /B-VI, JENDL4.0u and JEFF3.3, while the group lead by A. Hajii at CEA used the TRIPOLI and SERPENT Monte Carlo codes and JEFF-3.1.1, JEFF-3.2, ENDF/B-VIII, JENDL-4.0 and JEFF3.2 nuclear data libraries with neutron-scattering angular distributions for Fe56 from the JENDL evaluation. The focus was on identifying small discrepancies of the results of different benchmarks.

On this research topic a PhD thesis was concluded in September 2020 under the supervision of M. Hajii. I. A. Kodeli from the JSI was part of the thesis defence committee.

In 2020 we continued our active participation in the OECD/NEA working groups of the *International Reactor Physics Experiment Evaluation Project (IRPhEP)* and the *International Critical Safety Benchmark Evaluation Project (ICSBEP)*, in which we contributed a new evaluation of a reference experiment containing highly enriched uranium plates, moderated and reflected with Lucite. The experiment, which is important for uranium storage and transportation, was performed with the assistance of colleagues from the American Los Alamos National Laboratory, where the experiment was also performed. It is expected to be published in the 2021 ICSBEP Handbook.

In 2020 we collaborated within the European SANDA project. The JSI contributes work in several different areas, including the use of programs 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 close collaboration with EC-JRC and SCK • CEN we have finished the calculations, where the decay heat from PWR fuel assemblies was determined. A joint paper is in the preparation. Further collaboration is foreseen under the NEA OECD.

In the scope of a collaboration with the International Atomic Energy Agency (IAEA), we participated in a nuclear data evaluation within the International Network of Nuclear Data Evaluators INDEN "*https://www-nds.iaea.org/INDEN/*". In January 2020 the neutron dosimetry library IRDFF-II was released, which serves as the main reference in neutron dosimetry. Also, a paper was submitted for publication; it describes the evaluation of nuclear data for chromium isotopes. The new evaluations to a large extent solve the long-standing problem of the over-prediction of reactivity in reactor benchmarks that contain significant quantities of chromium or stainless steel.

During the COVID-19 pandemic there was a large demand for filtering facepiece respirators. Although such respirators are designed for single use the Covid-19 pandemic crisis made it necessary to seek for emergency alternatives. Recycling of single-use personal protective equipment is one such option, but requires appropriate and efficient sterilization procedures. In collaboration with other departments at the Jožef Stefan Institute we studied the sterilization options using gamma rays and high-energy electrons as well as the relation between the irradiation, particle removal efficiency and surface potential on the respirators.

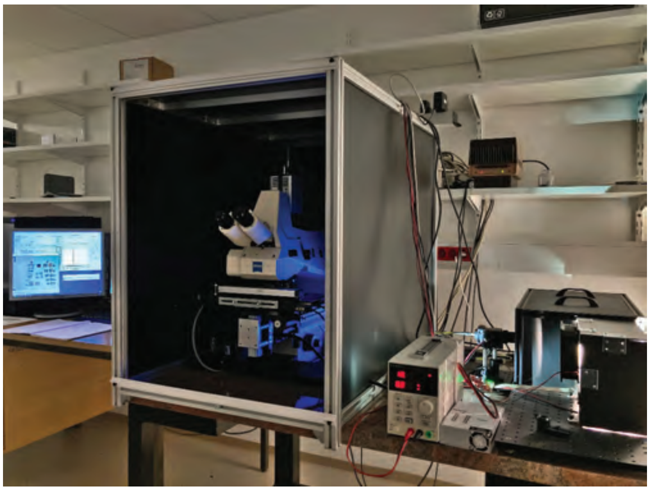

Figure 4: Laboratory for medical physics and microscopy. In the image is the custom hyperspectral microscope with control systems and a custom monochromatic light source.

Ionizing radiation has been identified as an option for the sterilization of disposable filtering facepiece respirators in situations where the production of the respirators cannot keep up with demand. Gamma radiation and high-energy electrons penetrate deep into the material and can be used to sterilize large batches of masks within a short time period. In relation to reports that sterilization by ionizing radiation reduces the filtration efficiency of polypropylene membrane filters on account of static charge loss, we have demonstrated that both gamma- and electron-beam irradiation can be used for sterilization, provided that the respirators are recharged afterwards. The results were published in the high-ranking Journal of Membrane Science.

The plasma section of the department continues its involvement in the endeavours of the EUROfusion Consortium. We have again been involved in several work packages (WPs) within its framework. In the WP MST1 we were a part of the international group studying the characteristics of filamentary transport in a tokamak in H-mode. Filamentary transport is predicted to be the main mode of transport in the scrape-off-layer (SOL) of the future large tokamaks, such as DEMO reactor. The emphasis was put on the different fuelling scenarios. We also contributed kinetic particle-in-cell (PIC) simulations using our further developed model, which we use to study the role of neutrals in the plasma transport processes. We have also contributed to the WP MST2, where we helped with the simulations of the thermal response of the so-called "New probe head" (NPH) to the plasma heat flux. The NPH is supposed to be the first instrument capable of measuring electron and ion temperatures at the same time at the same location and it will also feature the emissive probe, which is the only device capable of direct plasma potential measurements. Final calculations were made for repeated exposure of the NPH for the TCV and AUG tokamaks. Our work in the EUROfusion Enabling Research Project titled "Emissive divertor" involved the modelling of the inverted sheath using an analytical kinetic model and a kinetic PIC simulation model, which we both developed. The models proved to be in good agreement and can describe the range of the existence of the inverted sheath adequately. Some models predict the possibility of a highly emissive divertor in the future tokamaks, which would completely change the behaviour of the SOL plasma and consequently of the entire tokamak. We have also organized a small international experimental campaign on our linear magnetized plasma device in the frame of this project. The experiments tried to replicate the possibility of an electron emitting divertor in the tokamak using externally heated surfaces. Further experiments are planned for 2021. In collaboration with the IPP.CR and University of Sofia we have also completed a study on the effects of impurity seeding on the electron energy distribution function (EEDF) in the COMPASS tokamak. The EEDF can have a great effect on the heat loads to the surface and our task was to develop a model for calculating the energy flux to the divertor. We also contributed the interpretation of the phenomena of positive plasma potential in front of the surface.

In 2020 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 the 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 a comparison 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 the samples, which is a good starting point for similar future analyses in support of the future TT and DT campaigns at JET. Furthermore, in 2020 we also collaborated in the development of a methodology for the simulation of a gamma source and transport in the 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 which stared more than 20 year ago, specifically on 21–22 March 2000, when Slovenia joined the European fusion programme. In 2020 we contributed to a new experiment at FNG in Frascati called WCLL (Water Cooled Lithium Lead). The benchmark experiment was modelled using the XSUN-2017/SUSD3 code suite for particle transport and sensitivity and uncertainty analysis. Sensitivity and uncertainty analyses enable the optimization of measurements and the estimation of expected uncertainties. This enables the use of such experiments for nuclear data validation and improvement. On the basis of sensitivity and uncertainty information alongside a comparison of measured and calculated detector responses the quality of nuclear data can be assessed.

In 2021 we participated in several meetings and working groups at the OECD/NEA:

Working Party on International Nuclear Data Evaluation Co-operation (WPEC) Subgroup 46 in Subgroup 47 (SG46, SG47). The coordinator of the WPEC SG47 named "Using the complete SINBAD benchmark database for validation of nuclear data" is prof. Dr. Ivan A. Kodeli from the JSI. Two meetings were organized in 2020 in May and December. The goal of the work group is the further development of the SINBAD benchmark database. Measurement uncertainties of these experiments are typical much lower than the calculations, which gives the opportunity for nuclear data validation. The working group will finish its work in 2021.

Review Group Meeting IRPhE/ICSBEP/SINBAD (October 2020)

Meeting of the **EGRTS** group was held in February 2020. The topic of the meeting was neutron transport simulation and the SINBAD benchmark database.

Joint European Fission and Fusion File (**JEFF**): Meetings are held twice per year. This year we contributed work done on nuclear data within the EUROfusion project and JEFF dedicated work. In 2020 the reference publication for the JEFF-3.3 evaluated nuclear data library was published in The European Physical Journal A.

In 2020 we have successfully completed the project of dose-rates analyses due to the skyshine effect (backscattering of the particles in the air) on the demonstrational fusion reactor DEMO. As part of the project, we have determined the skyshine effect around the DEMO during the reactor operation, after shutdown and during the breeding blanket maintenance, where in the latter case, the highly activated part of the inner wall (breed blanket) was elevated to the upper maintenance hall. Analyses were performed using hybrid codes for neutral particle transport and programs developed at the JSI. Based on the performed analyses, we confirmed that the primary thickness of the shield is adequate, and in neither case the prescribed dose limits at the selected locations are not exceeded. By additional analysis of the shield thickness variation, the optimal thickness of the shield was determined. These analyses are an important part of the research to optimize the design of the future DEMO fusion reactor.

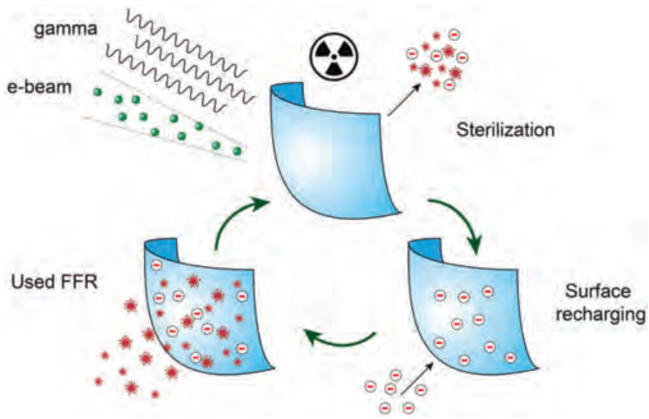

Figure 5: Ionizing radiation has been identified as an option for the sterilization of disposable filtering facepiece respirators in situations where the production of the respirators cannot keep up with demand. We have demonstrated that both gamma and electron beam irradiation can be used for sterilization, provided that the respirators are recharged afterwards.

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 2020 we continued with neutronics analyses in support of the design and development of the fusion power plant DEMO. In the first half of the year, we performed this work as part of the EUROfusion engineering grant and continued with it as a normal EUROfusion task in the second half of the year. The work included model preparation and testing of new DEMO reactor configurations with the emphasis on the nuclear heating of superconducting magnets and gamma fields around the reactor as a result of the integration of various systems. Analyses highlighted some of the suitable configurations and useful shielding strategies that will be taken into account in future models of the DEMO power plant. These analyses were an important part of the preparations to the design review that was performed towards the end of the preconceptual design phase at the end of 2020.

As in previous years we participated in the JET3-NEXP streaming benchmark experiment. This and last year, 2019, a new experimental camping in the so-called DD mode was conducted at JET. The experimental results from this campaign will be used for validation of simulation results of neutron fluence. The experiment was repeated using thermo-luminescent detectors 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. Six experimental locations were added to this camping. This year the JSI also contributed pre-analysis calculations for the TT and DT experimental campaigns. The TT and DT experiments will be conducted in 2021 and 2022.

In 2020 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 2020 the researcher continued in his 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 deuterium and, after almost 20 years, tritium plasmas. Through analyses performed with the TRANSP transport solver, we have analysed the effects of plasma heating on the fusion power produced and neutron emission properties, we have conducted studies of synergistic effects of the neutral beam injection and radiofrequency heating systems, as well as performed analyses of the effects of fast ions on plasma stability. Throughout the campaigns with deuterium plasma, we have conducted measurements of the activation of a set of In, Al and Fe foils, with which we have validated a recently developed computational chain for simulations of realistic neutron sources at JET.

In the field of **medical physics**, we focused mainly to the newly established field of biomedical optics. Here we continued our research of hyperspectral microscopy (HSM). We calibrated the technique spectrally and spatially. We performed the first imaging studies of tissue samples and histology and compared the results to the images obtained by conventional techniques. HSM was also a part of the PKP student project PoMIKRO, where HSM was used for imaging histology slides of eye melanoma. The students took RGB and HSM images and developed machine-learning algorithms for the classification of eye and tumour tissues. HSM was also explored in the context of doctoral work of Jošt Stergar, who will include the most important findings in his dissertation. We continued collaboration on analysis of hyperspectral images with colleagues from University of Rijeka.

In addition to that, we have continued our research in the areas that have been our main focus in the last few years: modelling, analysis of positron emission tomography (PET) images, and image-guided cancer therapy. We completed a prospective immunotherapy study conducted in collaboration with the Institute of Oncology Ljubljana, where patients with metastatic lung cancer were treated with anti-PD-1 immunotherapy (pembrolizumab) and imaged with computed tomography (CT) and fluorodeoxyglucose (FDG) PET/CT before treatment, as well as 1, 4, 10, 16 and 20 months after the treatment. We found that pre-treatment radiomics analyses of FDG PET/CT images correctly predicted patients' response to immunotherapy with 80% accuracy, which is much better than the current clinical standards. The manuscript has been published in a scientific journal.

We continued with the modelling of thermal transport for the purpose of thermography in medicine. Using a finger model that was developed last year (based on the MR image of the finger, 15 different structures), our research was mainly focused to mesh optimization in order to facilitate dynamic simulations and consequently to simulate stress tests (e.g., finger heat up after temporary immersion into cold water).

As always in recent years, we closely collaborated with the University of Wisconsin–Madison. The groups became even more organizationally integrated this year (weekly Zoom meetings, internal reviews of papers, etc.)

Some outstanding publications in the past year

1. Žohar, Andrej, Lengar, Igor, Snoj, Luka. Analysis of water activation in fusion and fission nuclear facilities. Fusion engineering and design. [Print ed.]. 2020, vol. 160, art. 111828, 17 str. ISSN 0920-3796. DOI: 10.1016/j.fusengdes.2020.111828. [COBISS.SI-ID 20616195]
2. Radulović, Vladimir, Jaćimović, Radojko, Pungerčič, Anže, Vavtar, Ingrid, Snoj, Luka, Trkov, Andrej. Characterization of the neutron spectra in three irradiation channels of the JSI TRIGA reactor using the GRUPINT spectrum adjustment code. Nuclear data sheets. 2020, vol. 167, july-august, str. 61-75. ISSN 0090-3752. DOI: 10.1016/j.nds.2020.07.003. [COBISS.SI-ID 25625091]
3. Stergar, Jošt, Dolenec, Rok, Kojc, Nika, Lakota, Katja, Perše, Martina, Tomšič, Matija, Milanič, Matija. Hyperspectral evaluation of peritoneal fibrosis in mouse models. Biomedical optics express. 2020, vol. 11, iss. 4, str. 1991-2006, ilustr. ISSN 2156-7085. DOI: 10.1364/BOE.387837. [COBISS.SI-ID 3414372], [JCR, SNIP, WoS do 13. 9. 2020: št. citatov (TC): 1, čistih citatov (CI): 1, Scopus]
4. Naglič, Peter, Zelinskyi, Yevhen, Rogelj, Luka, Stergar, Jošt, Milanič, Matija, Novak, Jure, Kumperščak, Borut, Bürmen, Miran. Optical properties of PlatSil SiliGlass tissue-mimicking phantoms. Biomedical optics express. 1 Jul. 2020, vol. 11, no. 7, str. 3753-3768, ilustr. ISSN 2156-7085. https://www.osapublish-

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5. Valentinuzzi, Damijan, Vrankar, Martina, Boc, Nina, Ahac, Valentina, Zupančič, Žiga, Unk, Mojca, Škalič, Katja, Žagar, Ivana, Studen, Andrej, Simončič, Urban, Eickhoff, Jens C., Jeraj, Robert. [18F]FDG PET immunotherapy radiomics signature (iRADIOMICS) predicts response of non-small-cell lung cancer patients treated with pembrolizumab. Radiology and oncology. [Print ed.]. 2020, vol. 54, iss. 3, str. 285-294, ilustr. ISSN 1318-2099. DOI: 10.2478/raon-2020-0042. [COBISS.SI-ID 24723203], [JCR, SNIP, WoS do 14. 11. 2020: št. citatov (TC): 1, čistih citatov (CI): 1, Scopus]
6. Plompen, A.J.M., Cabellos, O., Saint-Jean, C. De, Fleming, M., Algora, A., Angelone, M., Archier, P., Bauge, E., Bersillon, O., Kodeli, Ivan Aleksander, Kos, Bor, Trkov, Andrej, Žerovnik, Gašper, et al. The joint evaluated fission and fusion nuclear data library, JEFF-3.3. European physical journal. A, Hadrons and nuclei. 2020, vol. 56, art. 181, 108 str. ISSN 1434-601X. DOI: /10.1140/epja/s10050-020-00141-9. [COBISS.SI-ID 22761219]
7. Kos, Bor, Sjostrand, H., Kodeli, Ivan Aleksander, Čufar, Aljaž, Drenik, Aleksander, Lengar, Igor, Štancar, Žiga, Snoj, Luka, et al., JET Contributors. Nuclear data uncertainty propagation in complex fusion geometries. Journal of nuclear engineering. 2020, vol. 1, no. 1, str. 63-69. ISSN 2673-4362. DOI: /10.3390/jne1010006. [COBISS.SI-ID 41490947]
8. A. Trkov, P.J. Griffin, S.P. Simakov, L.R. Greenwood, K.I.Zolotarev, R. Capote, D.L. Aldama, V. Chechev, C. Destouche, A.C. Kahler, C. Konno, M.Koštál, M.Majerle, E. Malambum, M. Ohta, V.G. Pronyaev, V. Radulović, S. Saton ... H. Yashimas, IRDFF-II: A New Nevtron Metrology Library, Nuclear Data Sheets, Volume 163, January 2020, Pages 1-108

Awards and Appointments

1. Bor Kos: Best Poster Award, Portorož, Slovenia, 29th International Conference Nuclear Energy for New Europe - NENE 2020, September 2020, for a poster TCV Tokamak Neutron Shielding Assessment and UpgradeDomen Kotnik: Faculty Prešeren Award for MSc Thesis, Ljubljana, University of Ljubljana, Faculty of Mathematics and Physics, January 2020 (more at: KOTNIK, Domen. Validacija in praktična uporaba programa za transport nevtronov in fotonov ADVANTG : magistrsko delo. Ljubljana: [D. Kotnik], 2019. XVI, 134 str., ilustr. https://repozitorij.uni-lj.si/IzpisGradiva.php?id=107756&lang=slv. [COBISS.SI-ID 3313508] nagrada: Prešernova nagrada študentom Fak. za matematiko in fiziko za l. 2020)
2. Andrej Žohar: Young Author Award for the best contribution, Portorož, Slovenia, 29th International Conference Nuclear Energy for New Europe - NENE 2020, September 2020, for an article Water Activation Experiment and Calculations at JSI TRIGA Research Reactor

Organization of Conferences, Congresses and Meetings

1. 29th International Conference Nuclear Energy for New Europe - NENE 2020, Portorož, Slovenia, 7. 9.–10. 9. 2020, organizer (conference in hybrid format)

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. Training Fees for Mr. Eyakifama Hazou, ICTP-IAEA Sandwich Training Educational Programme (STEP), from 16 February 2019 to 16 May 2019
   Prof. Luka Snoj
   Ictp - Centro Internazionale Di Fisica Teorica
5. 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
6. H2020 - EURAD; European Joint Programme on Radioactive Waste Management
   Dr. Vladimir Radulović
   European Commission
7. H2020 - ENEEP; European Nuclear Experimental Educational Platform
   Dr. Vladimir Radulović
   European Commission
8. H2020 - SANDA; Supplying Accurate Nuclear Data for Energy and Non-Energy Applications
   Prof. Ivan Aleksander Kodeli
   European Commission
9. H2020 - ARIEL; Accelerator and Research Reactor Infrastructures for Education and Learning
   Prof. Ivan Aleksander Kodeli
   European Commission
10. H2020 - TOURR; Towards Optimized Use of Research Reactors in Europe
    Prof. Luka Snoj
    European Commission
11. H2020 - EUROfusion; Research Unit - Administration and Services RU – FU
    Prof. Luka Snoj
    European Commission
12. H2020 - EUROfusion; Enabling Research-2-FU
    Dr. Jernej Kovačič
    European Commission
13. H2020 - EUROfusion; Exploatation of DT Operation for ITER-JET3-FU
    Prof. Luka Snoj
    European Commission
14. H2020 - EUROfusion; Education-ED-FU
    Prof. Luka Snoj
    European Commission
15. H2020 - EUROfusion; JET Campaigns-JET1-2021-C40

Dr. Žiga Štancar
European Commission
16. H2020 - EUROfusion; Medium Size Tokamak Campaigns-MST1-FU
Dr. Jernej Kovačič
European Commission
17. H2020 - EUROfusion; Preparation and Exploitation of Medium Size Tokamaks - WPMST2-FU
Dr. Jernej Kovačič
European Commission
18. H2020 - EUROfusion; PMI-PPPT-2-FU: Nuclear data
Prof. Ivan Aleksander Kodeli
European Commission
19. H2020 - EUROfusion; Engineering Grants: Fusion Plant Nuclear Analyst - The modelling of the proposed DEMO component designs, testing their performance under reactor conditions and development of new design solutions
Dr. Aljaž Čufar
European Commission
20. Multiphysics Validation of High Fidelity Modelling and Simulation for Nuclear Applications
Dr. Vladimir Radulović
Slovenian Research Agency
21. Use of Shielding Benchmarks for Nuclear Data Validation and Improvement
Prof. Ivan Aleksander Kodeli
Slovenian Research Agency
22. Optimization of Neutron Converting Components for Enhanced Performance of Silicon Carbide Based Neutron Detectors
Prof. Luka Snoj
Slovenian Research Agency
23. 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
24. Development of Multiphysics Tools for Plasma and Neutron Transport Calculations in Modern Fusion Devices
Dr. Žiga Štancar
Slovenian Research Agency
25. 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

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. Analysis of nuclear heating in a reactor
Prof. Luka Snoj
2. Determination of the Am-241 thermal neutron capture cross section by activation measurements at the JSI TRIGA reactor
Dr. Gašper Žerovnik
3. Contribution to the improvement of nuclear data for higly reliable reactor shielding calculations
Prof. Ivan Aleksander Kodeli
4. Absolute radiation measurements at very high neutron flux levels in reactor pulse mode
Prof. Igor Lengar
5. Electrocaloric elements for active cooling of electronic circuits
Prof. Luka Snoj
6. Advances in Thermal Scattering Law Analysis
Prof. Luka Snoj
7. Experimental Benchmark for validation of the modelling of neutron and gamma instrumentation
Dr. Vladimir Radulović
8. Sensitivity of nuclear reactor physical parameters to thermal nuclear data
Prof. Andrej Trkov
9. Development of Computational Tools for the Determination of the Neutron Field in the Containment of a Pressurized Water Reactor
Prof. Andrej Trkov
10. Stability of nuclear reactors in load follow mode of operation
Prof. Luka Snoj
11. Fusion for Energy - F4E
Prof. Igor Lengar
Ministry of Education, Science and Sport
12. ICERR Agreement for Receiving Affiliate Staff to CEA as a Designated International Center based on Research Reactors, through its Research Centres of Saclay and Cadarache
Prof. Luka Snoj
CEA - Commissariat A L"energie Atomique Et Aux
13. Irradiation of Glycol
Prof. Luka Snoj
Lancaster University
14. Irradiations on the TRIGA Reactor
Prof. Luka Snoj
15. Neutron Transport and Criticality Calculations in Reactor Cores
Dr. Vladimir Radulović
Institut de Radioprotection et de Surete Nucleaire
16. Pre-design MCNP Calculations for the TCV Neutron Shielding
Dr. Bor Kos
EPFL/SB/SPC
17. Irradiations of FT-TIMS Capsule on the TRIGA Reactor for Years 2020-2022
Prof. Luka Snoj
CEA-commissariat a l' Energie Atomique et aux

NEW CONTRACTS

1. Independent Evaluation of the report „KRŠKO - Assessment of Increased Cycle Burnup for Reload Safety Evaluation"
Asst. Prof. Marjan Kromar
Nuklearna Elektrarna Krško d. o. o.
2. Optimization of storage in dry storage containers – SFDS
Asst. Prof. Marjan Kromar
Nuklearna Elektrarna Krško d. o. o.
3. Support for reviews and calculations in the SFDS project for 2020 and 2021
Prof. Luka Snoj
Nuklearna Elektrarna Krško d. o. o.
4. 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.

VISITORS FROM ABROAD

1. Dr Takihiro Makino, QST - National Institutes for Quantum and Radiological Science and Technology, Takasaki, Anagawa, Japan, 3. 2.–7. 2. 2020
2. Arran Plant, Lancaster University, Engineering Department, Lancaster, United Kingdom, 17. 2.–21. 2. 2020
3. Dr Aidan Reilly, United Kingdom Atomic Energy Authority, Abingdon, United Kingdom, 20.2.–21. 2. 2020
4. Dr James P. Gunn, Institut de Recherches sur la Fusion Magnétique, Saint Paul Lez Durance, France, 24. 2.–6. 3. 2020
5. Prof. Tsviatko K. Popov, University "St. Kliment Ohridski", Faculty of Physics, Sofia, Bulgaria, 24. 2.–6. 3. 2020
6. Dr Daniel de A.M. Campolina, Nuclear Technology Development Centre, Belo Horizonte, MG, Brazil, 7. 3.–3. 4. 2020
7. Serhii Kupriianchuk, Institute for Safety Problems of NPPs, Ukraine's National Academy of Sciences, Kyiv, Ukraine, 7. 3.–7. 6. 2020

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Researchers
1. Dr. Dušan Čalič
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4. Prof. Ivan Aleksander Kodeli
5. Asst. Prof. Marjan Kromar
6. Prof. Igor Lengar
7. Asst. Prof. Matija Milanič*

8. Dr. Vladimir Radulović
9. Dr. Urban Simončič*
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11. Prof. Andrej Trkov
12. Dr. Gašper Žerovnik

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13. Stefan Costea, B. Sc.
14. Dr. Aljaž Čufar
15. Dr. Bor Kos
16. Dr. Jernej Kovačič
17. *Dr. Vid Merljak, left 21.01.20*
18. Dr. Žiga Štancar

Postgraduates

19. *Klemen Ambrožič, B. Sc., left 16.05.20*
20. Tanja Goričanec, B. Sc.
21. Domen Kotnik, B. Sc.
22. Jan Malec, B. Sc.
23. Stefano Marciano, B. Sc.
24. Anže Pungerčič, B. Sc.
25. Ingrid Švajger, B. Sc.
26. *Dr. Damijan Valentinuzzi, left 02.11.20*
27. Andrej Žohar, B. Sc.

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28. Slavko Slavič, B. Sc.
29. Saša Škof, B. Sc.
30. Bojan Žefran

Note:
* part-time JSI member

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Original Article

1. Domen Kotnik, Bor Kos, Dušan Ćalić, Luka Snoj, "Use of ADVANTG to analyse skyshine γ-dose rates around a silo type LILW repository", *Annals of Nuclear Energy*, 2020, **145**, 107585.
2. Jan Malec, Dan Toškan, Luka Snoj, "PC-based JSI research reactor simulator", *Annals of Nuclear Energy*, 2020, **146**, 107630.
3. Marcella Cagnazzo *et al.* (16 authors), "The European nuclear experimental educational platform (ENEEP) for education and training", *Atw. Internationale Zeitschrift für Kernenergie*, 2020, **65**, 5, 251-256.
4. Jošt Stergar, Rok Dolenec, Nika Kojc, Katja Lakota, Martina Perše, Matija Tomšič, Matija Milanič, "Hyperspectral evaluation of peritoneal fibrosis in mouse models", *Biomedical optics express*, 2020, **11**, 4, 1991-2006.
5. Peter Naglič, Yevhen Zelinskyi, Luka Rogelj, Jošt Stergar, Matija Milanič, Jure Novak, Borut Kumperščak, Miran Bürmen, "Optical properties of PlatSil SiliGlass tissue-mimicking phantoms", *Biomedical optics express*, 2020, **11**, 7, 3753-3768.
6. Tomislav Brodar, Luka Bakrač, Ivana Capan, Takeshi Ohshima, Luka Snoj, Vladimir Radulović, Željko Pastuović, "Depth profile analysis of deep level defects in 4H-SiC introduced by radiation", *Crystals*, 2020, **10**, 845-861.
7. A.J.M. Plompen *et al.* (80 authors), "The joint evaluated fission and fusion nuclear data library, JEFF-3.3", *European physical journal. A, Hadrons and nuclei*, 2020, **56**, 181.
8. Ivan Aleksander Kodeli, Aljaž Čufar, "Validation of DT source term modelling in MCNP and MCUNED codes against SINBAD fusion benchmarks", *Fusion engineering and design*, 2020, **154**, 111542.
9. S. Garavaglia *et al.* (15 authors), "EU DEMO EC equatorial launcher pre-conceptual performance studies", *Fusion engineering and design*, 2020, **156**, 111594.
10. Boštjan Končar, Martin Draksler, Jernej Kovačič, Bernd Sebastian Schneider, Codrina Ioniţă, Tomaž Gyergyek, Cedric Kar-Wai Tsui, Roman Schrittwieser, "Analysis of thermal response of new diagnostic probe in TCV", *Fusion engineering and design*, 2020, **156**, 111744.
11. Aljaž Čufar, Christian Bachmann, T. Eade, D. Flammini, C. Gliss, Ivan Aleksander Kodeli, Domenico Marzullo, Giuseppe Mazzone, C. Vorpahl, A. Wilde, "Shielding concept and neutronic assessment of the DEMO lower remote handling and pumping ports", *Fusion engineering and design*, 2020, **157**, 111615.
12. Thomas Franke *et al.* (14 authors), "The EU DEMO equatorial outboard limiter - design and port integration concept", *Fusion engineering and design*, 2020, **158**, 111647.
13. Andrej Žohar, Igor Lengar, Luka Snoj, "Analysis of water activation in fusion and fission nuclear facilities", *Fusion engineering and design*, 2020, **160**, 111828.
14. P. Spaeh, Christian Bachmann, R. Chavan, Aljaž Čufar, Thomas Franke, Dirk Strauss, Minh Quang Tran, "Structural pre-conceptual design studies for an EU DEMO equatorial EC port plug and its port integration", *Fusion engineering and design*, 2020, **161**, 111885.
15. Andrej Žohar, Anže Pungerčič, Klemen Ambrožič, Vladimir Radulović, Igor Lengar, Luka Snoj, "Analysis of irradiation experiments with activated water radiation source at the JSI TRIGA Research Reactor", *Fusion engineering and design*, 2020, **161**, 111946.
16. R. Worrall, Bethany Colling, M. R. Gilbert, E. Litherland-Smith, C. R. Nobs, L. W. Packer, C. Wilson, Andrej Žohar, "The development, testing and comparison of unfolding methods in SPECTRA-UF for neutron spectrometry", *Fusion engineering and design*, 2020, **161**, 112038.
17. Boštjan Končar, Oriol Costa Garrido, Martin Draksler, A. Herrmann, Jernej Kovačič, Codrina Ioniţă, Roman Schrittwieser, "Analysis of thermal and structural responses of a new diagnostic probe to repeated exposure in ASDEX upgrade tokamak", *Fusion engineering and design*, 2020, **161**, 112047.
18. Adrien Gruel, Klemen Ambrožič, Christophe Destouches, Vladimir Radulović, A. Sardet, Luka Snoj, "Gamma-heating and Gamma flux measurements in the JSI TRIGA Reactor: results and prospects", *IEEE transactions on nuclear science*, 2020, **67**, 4, 559-567.
19. Bor Kos, Henrik Sjostrand, Ivan Aleksander Kodeli and JET Contributors, "Nuclear data uncertainty propagation in complex fusion geometries", *Journal of nuclear engineering*, 2020, **1**, 1, 63-69.
20. Andrej Trkov *et al.* (24 authors), "IRDFF-II: A new neutron metrology library", *Nuclear data sheets*, 2020, **163**, 1-108.
21. Vladimir Radulović, Radojko Jaćimović, Anže Pungerčič, Ingrid Vavtar, Luka Snoj, Andrej Trkov, "Characterization of the neutron spectra in three irradiation channels of the JSI TRIGA reactor using the GRUPINT spectrum adjustment code", *Nuclear data sheets*, 2020, **167**, 61-75.
22. the ASDEX Upgrade Team, the TCV Team and the EUROfusion MST1 Team, Nicola Vianello *et al.*, "Scrape-off layer transport and filament characteristics in high-density tokamak regimes", *Nuclear fusion*, 2020, **60**, 1, 016001.
23. V.G. Kiptily *et al.* (16 authors) and JET Contributors, "Excitation of elliptical and toroidal Alfvén Eigenmodes by ^{3}He-ions of the MeV-energy range in hydrogen-rich JET plasmas", *Nuclear fusion*, 2020, **60**, 11, 112003.
24. Yevgen Kazakov *et al.* (22 authors) and JET Contributors, "Plasma heating and generation of energetic D ions with the 3-ion ICRF + NBI scenario in mixed H-D plasmas at JET-ILW", *Nuclear fusion*, 2020, **60**, 11, 112013.
25. Massimo Nocente *et al.* (47 authors) and JET Contributors, "Generation and observation of fast deuterium ions and fusion-born alpha particles in JET D- 3He plasmas with the 3-ion radio-frequency heating scenario", *Nuclear fusion*, 2020, **60**, 12, 124006.
26. Ivana Capan, Tomislav Brodar, Yuichi Yamazaki, Yuya Oki, Takeshi Ohshima, Yoji Chiba, Yasuto Hijikata, Luka Snoj, Vladimir Radulović, "Influence of neutron radiation on majority and minority carrier traps in n-type 4H-SiC", *Nuclear instruments & methods in physics research. Section B, Beam interactions with materials and atoms*, 2020, **478**, 224-228.
27. Vladimir Radulović *et al.* (11 authors), "Silicon carbide neutron detector testing at the JSI TRIGA reactor for enhanced border and port security", *Nuclear instruments and methods in physics research. Section A, Accelerators, spectrometers, detectors and associated equipment*, 2020, **972**, 164122.
28. Gregor Kramberger, Klemen Ambrožič, U. Gürer, Bojan Hiti, H. Karacali, Igor Mandić, E. Yilmaz, O. Yilmaz, Marko Zavrtanik, "Development of MOS-FET dosimeters for use in high radiation fields", *Nuclear*

instruments and methods in physics research. Section A, Accelerators, spectrometers, detectors and associated equipment, 2020, **978**, 164283.
29. Tomaž Gyergyek, Jernej Kovačič, Iñaki Gómez Alonso, James Paul Gunn, Stefan Costea, Miran Mozetič, "Kinetic model of an inverted sheath in a bounded plasma system", *Physics of plasmas*, 2020, 2, 023520.
30. the COMPASS team and the EUROfusion MST1 Team, Miglena Dimitrova *et al.*, "Impact of impurity seeding on the electron energy distribution function in the COMPASS divertor region", *Plasma physics and controlled fusion*, 2020, **62**, 12, 125015.
31. Klemen Ambrožič, Luka Snoj, "JSIR2S code for delayed radiation simulations: Validation against measurements at the JSI TRIGA reactor", *Progress in Nuclear Energy*, 2020, **129**, 103498.
32. Anže Pungerčič, Dušan Ćalić, Luka Snoj, "Computational burnup analysis of the TRIGA Mark II research reactor fuel", *Progress in Nuclear Energy*, 2020, **130**, 103536.
33. Damijan Valentinuzzi *et al.* (12 authors), "[^{18}F]FDG PET immunotherapy radiomics signature (iRADIOMICS) predicts response of non-small-cell lung cancer patients treated with pembrolizumab", *Radiology and oncology*, 2020, **54**, 3, 285-294.

Review Article

1. Damijan Valentinuzzi, Robert Jeraj, "Computational modelling of modern cancer immunotherapy", *Physics in Medicine & Biology*, 2020, **65**, 24tr01.

Published Conference Contribution (invited lecture)

1. J. Y. Ferrandis, O. Gatsa, P. Combette, D. Fourmentel, Christophe Destouches, Vladimir Radulović, Luka Snoj, "Acoustic instrumentation of the new generation of MTR: effect of nuclear radiation on modified Bismuth Titanate piezoelectric elements", In: *ANIMMA 2019, Advancements in Nuclear Instrumentation Measurement Methods and their Applications, June 17-21, 2019, Portorož, Slovenia*, Proceedings, (EPJ Web of Conferences **225**), EDP Sciences, 2020, 04012.
2. Luka Snoj *et al.* (22 authors), "Radiation hardness studies and detector characterisation at the JSI TRIGA reactor", In: *ANIMMA 2019, Advancements in Nuclear Instrumentation Measurement Methods and their Applications, June 17-21, 2019, Portorož, Slovenia*, Proceedings, (EPJ Web of Conferences **225**), EDP Sciences, 2020, 04031.

Published Conference Contribution

1. Iñaki Gómez Alonso, Anej Valič, Tomaž Gyergyek, Stefan Costea, Jernej Kovačič, "Particle-in-cell simulations of an inverted sheath", In: *21st International Summer School on Vacuum, Electron and Ion Technologies, 23-27 September 2019, Sozopol, Bulgaria*, Proceedings, (Journal of Physics: Conference Series **1492**), IOP Publishing, 2020, 012004.
2. Bor Kos, Theodora Vasilopoulou, Scott W. Mosher, Ivan Aleksander Kodeli, Robert E. Grove, Jonathan Naish, Barbara Obryk, Rosaria Villari, Paola Batistoni and JET Contriburtors, "Analysis of DD, TT and DT neutron streaming experiments with the ADVANTG code", In: *ANIMMA 2019, Advancements in Nuclear Instrumentation Measurement Methods and their Applications, June 17-21, 2019, Portorož, Slovenia*, Proceedings, (EPJ Web of Conferences **225**), EDP Sciences, 2020, 02003.
3. Aljaž Čufar *et al.* (13 authors) and JET Contributors, "Detailed reproduction of the neutron emission from the compact DT neutron generator used as an in-situ 14 MeV calibration neutron source at JET", In: *ANIMMA 2019, Advancements in Nuclear Instrumentation Measurement Methods and their Applications, June 17-21, 2019, Portorož, Slovenia*, Proceedings, (EPJ Web of Conferences **225**), EDP Sciences, 2020, 02005.
4. Tanja Goričanec, Domen Kotnik, Žiga Štancar, Luka Snoj, Marjan Kromar, "Predicting ex-core detector response in a PWR with Monte Carlo neutron transport methods", In: *ANIMMA 2019, Advancements in Nuclear Instrumentation Measurement Methods and their Applications, June 17-21, 2019, Portorož, Slovenia*, Proceedings, (EPJ Web of Conferences **225**), EDP Sciences, 2020, 03007.
5. Andrej Žohar, Anže Pungerčič, Klemen Ambrožič, Vladimir Radulović, Anže Jazbec, Sebastjan Rupnik, Igor Lengar, Luka Snoj, "Conceptual design of irradiation facility with 6 MeV and 7 MeV gamma rays at the JSI TRIGA Mark II research reactor", In: *ANIMMA 2019, Advancements in Nuclear Instrumentation Measurement Methods and their Applications, June 17-21, 2019, Portorož, Slovenia*, Proceedings, (EPJ Web of Conferences **225**), EDP Sciences, 2020, 04014.
6. Igor Lengar, Sebastjan Rupnik, Andrej Žohar, Vid Merljak, Marjan Kromar, Luka Snoj, "Usage of multiple fission cells for neutron flux measurements during rod-insertion method", In: *ANIMMA 2019, Advancements in Nuclear Instrumentation Measurement Methods and their Applications, June 17-21, 2019, Portorož, Slovenia*, Proceedings, (EPJ Web of Conferences **225**), EDP Sciences, 2020, 04024.
7. Ingrid Vavtar, Anže Pungerčič, Luka Snoj, "Utilisation of JSI TRIGA pulse experiments for testing of nuclear instrumentation and validation of transient models", In: *ANIMMA 2019, Advancements in Nuclear Instrumentation Measurement Methods and their Applications, June 17-21, 2019, Portorož, Slovenia*, Proceedings, (EPJ Web of Conferences **225**), EDP Sciences, 2020, 04027.
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THESES AND MENTORING

1. Klemen Ambrožič, *Characterization of gamma field in the JSI TRIGA reactor:* doctoral dissertation, Ljubljana, 2020 (mentor Luka Snoj).
2. Anže Jazbec, *Calculation of gamma and neutron dose field inside the JSI TRIGA Mark II reactor hall:* doctoral dissertation, Ljubljana, 2020 (mentor Luka Snoj).
3. Bor Kos, *Use of hybrid methods for neutron transport and sensitivity analysis:* doctoral dissertation, Ljubljana, 2020 (mentor Ivan A. Kodeli; co-mentor Scott W. Mosher).
4. Damijan Valentinuzzi, *Physical models of immunotherapy:* doctoral dissertation, Ljubljana, 2020 (mentor Robert Jeraj).

DEPARTMENT OF EXPERIMENTAL PARTICLE PHYSICS F-9

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

Report on activities in 2020

In order to reveal the ultimate secrets of nature in the world of elementary particles, accelerators with higher and higher energies are needed. Their cost, both in terms of money and human resources, has grown to the level where they are affordable only as joint international enterprises. Thus, future accelerators will be unique facilities of their kind. 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 (750 researchers, 101 institutions from 22 countries)

The European Research Council (ERC) awarded an advanced grant to the project "Flavour Anomalies with advanced particle Identification Methods (FAIME)" proposed by our department in which data collected with the Belle II detector will be analysed

In the field of astroparticle physics we are part of the Pierre Auger collaboration (250 researchers, 94 institutions from 17 countries), which uses a giant scale (3000 km^2) 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 2020 activities follows, focused on the contributions of our researchers.

ATLAS experiment

In the last two years an upgrade has been taking place at CERN, as the Large Hadron Collider (LHC), as well as its detectors, is being upgraded before the next re-start, which gives us the much-needed time to analyse the data collected so far. The years 2015–2018 at CERN are the data-taking period of the Large Hadron Collider (LHC) named "Run 2". In 2015 the upgraded LHC began its operation 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 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 led to the most precise Run 2 searches of new physics beyond the Standard model hitherto achieved (figure 1). In the analysed data 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

- **In the analysed data 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.**
- **High-Granularity Timing Detector (HGTD) will be a part of ATLAS upgrade for the High-Luminosity LHC upgrade. The JSI group has taken a large part in the development of the Low Gain Avalanche Detectors (LGAD) for the HGTD.**

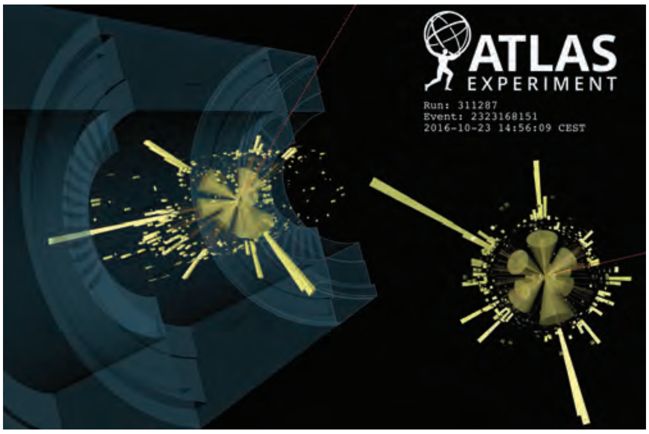

Figure 1: Event display visualisation of the highest jet multiplicity event selected in signal regions targeting long cascade decays of pair-produced gluinos. This event was recorded by ATLAS on 23 October 2016, and contains 16 jets, illustrated by cones. Yellow blocks represent the calorimeter energy measured in noise-suppressed clusters.

Standard Model, were excluded and there are some indications for potential new discoveries in particle physics – but for confirming or refuting these the full set of recorded data needs to be analysed. Subsequently, the next year will still be full of challenges and expectations of pivotal events. In 2020 the ATLAS collaboration published more than 70 scientific papers in the most distinguished scientific journals, bringing the total number of scientific papers published by the collaboration to 970, with more than a hundred further papers in preparation. Some of the outstanding papers published last year are listed below [1-4].

The ATLAS Ljubljana group had a leading role in designing, building and operating several beam- and radiation-monitoring systems, namely: ATLAS Beam Condition Monitor (BCM), Beam Loss Monitor (BLM), Radiation Monitor (RADMON) and Diamond Beam Monitor (DBM). The BCM was built to monitor conditions of the LHC beams and issue warnings at 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 the ATLAS Inner Detector from potential damage by LHC beams. 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. DBM was installed during the last shutdown and was used for the first time in 2015. It is built from pCVD diamond sensor and pixel readout chip with pixels of size 250×50 um^2. It can provide luminosity measurement complementary to the BCM and other luminosity monitors in ATLAS. Its readout was first tested during the last operation with beams.

Atlas detector upgrade

In 2020 the LHC was preparing for the new 2-year-long data-taking period "Run 3", starting in 2022. After Run 3 a major upgrade of LHC to High Luminosity LHC (HL-LHC) will start and the beginning of operation is scheduled for 2027. To adapt to the HL-LHC conditions a major upgrade of the ATLAS detector will be made. A large part of the ATLAS collaboration, including the group from the F9 department is intensively working on developing and building detector systems for the upgrade.

The group from the F9 department has taken a leading role in the development of a new system to replace the current beam abort and luminosity monitors based on pCVD diamond sensors. A dedicated rad-hard ASIC readout chip for the new system has been developed, which will be used to amplify and discriminate the signals coming from a segmented pCVD diamond sensor. We are currently in the phase of verifying the radiation hardness of individual components and planning the final architecture of the system.

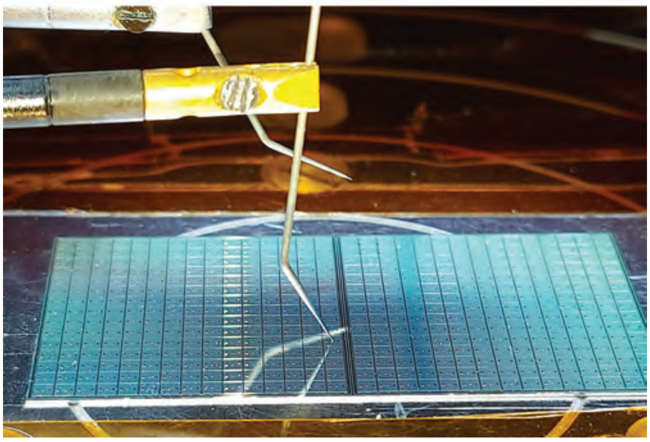

Figure 2: A large multi-channel LGAD (15×30 pads) which can achieve 25-ps time and 375-μm position resolution for fast charged particles during testing.

The High Granularity Timing Detector has officially become part of an ATLAS upgrade for the High-Luminosity LHC upgrade. The JSI group has played a large part in the development and testing of suitable Low Gain Avalanche Detectors LGADs (figure 2) for the HGTD, as documented in publications [5-10]. 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 to radiation hardness of the LGADs, particularly a reduced acceptor removal. The effective inter-pad distance in multi-electrode sensors were systematically measured using Scanning-TCT technique.

First, we thoroughly measured the effects of annealing on the sensor performance and showed that the radiation damage in LGADs does not depend on the neutron flux.

In 2020, the ATLAS collaboration began assembling components to upgrade the inner tracking detector (Inner tracker – ITk). Silicon microstrip sensors will be used to track the path of charged particles. It is estimated that in the first pre-series production phase we will assemble about 5% of the components. Our group participates in the process of ensuring the quality of sensors (QA). At the Reactor Center in Podgorica, we will irradiate test structures made on silicon wafers with neutrons. Regular irradiations are planned every month for a period of 4 years. In a specially designed measuring system, we measure the response of sensors with the help of the Sr^{90} source and the

ALIBAVA multi-channel readout system. All sensors from the pre-series show the expected degradation of the signals, the signal is reduced to about a third after irradiation with 1.6 10^{15} $n_{eq}cm^{-2}$, this corresponds to about 7500 electrons. Measurements on pre-series sensors showed the expected results.

In addition to the sensors' development we took part in special multilayer flexible circuit development together with company Elgoline d.o.o. The circuit connects the sensors with peripheral read-out electronics and power for HGTD. The first prototypes were produced in 2020. In collaboration with Elgoline d.o.o. multilayer large dimension flexible circuits were also developed for ITk and their production has started recently. Together with Oxford University a robot (figure 3) for testing of these circuits was developed. Elgoline from Cerknica will produce more than 1000 such large flexible circuits needed for the assembly of two endcaps of ITk. Each circuit will be tested three times in different stages of the assembly process.

A system for online measurements of integrated doses (RadMon) will be installed in the ITk. In 2020 our group designed and manufactured a prototype of a ceramic printed circuit, sensors for measurements of ionizing doses (RadFETs) were tested and selected and the design of the readout circuitry was started.

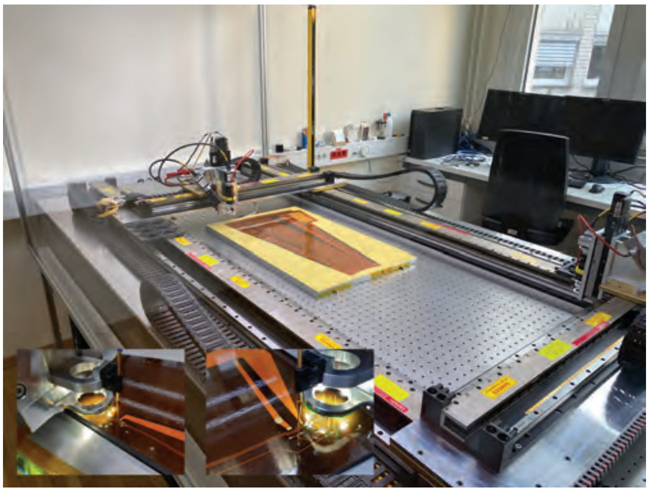

Figure 3: The figure shows two movable test stations, parts of the robot, with which the robot makes electrical contact with the circuit and measures its properties and detects any irregularities.

- **In the extensions of the SM a new gauge boson Z' could explain some discrepancies between the theoretical predictions and experimental results in measurements of $B \rightarrow K^{(*)} l^+ l^-$ decays, as well as the composition of the dark matter.**
- **European Research Council (ERC) awarded an Advanced Grant to the FAIME project, led by prof. dr. Peter Križan.**
- **In the FAIME project we will try to confirm or refute the preliminary results showing that under certain conditions tau leptons behave slightly differently than muons and electrons. Confirmation would mean a major revolution in elementary particle physics and in our understanding of nature in general.**

Belle detector at the asymmetric electron positron collider KEKB at K

Collaborators at the department continued activities at the Belle (Belle II) experiment on the electron-positron collider KEKB (SuperKEKB) in Tsukuba, Japan. The main motivation of 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 in order 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 others – for the observed dominance of matter over antimatter in the Universe.

Detector Belle finished data-taking in 2010. Numerous analyses of the data, however, are still in progress. Among the results of 2020 is the search for a hypothetical new gauge boson Z' [11] (Figure 4). In the extensions of the SM the latter could be responsible for some discrepancies between the theoretical predictions and experimental results in measurements of $B \rightarrow K^{(*)} l^+ l^-$ decays, as well as for the composition of dark matter.

Another high-impact result of the Belle collaboration in 2020 was a new test of lepton flavour universality through the measurement of $B \rightarrow D^* \tau\nu$ [12]. The measurement was performed using the so-called Full Event Interpretation in which one of the B mesons, produced in $e^+e^- \rightarrow \Upsilon(4S) \rightarrow BB$bar, is reconstructed through its semi-leptonic decays $B \rightarrow X_c l\nu$ (where X_c denotes any hadronic system composed of a c quark). This enables a determination of the energy and momentum of the other B meson decaying into $D^* \tau\nu$ (τ lepton further decays into a charged particle and one or more neutrinos). Despite the presence of at least two undetected neutrinos in the final state the method enables reconstruction of semi-tauonic decays and by this comparison of their rate to the rate of semi-leptonic decays into electrons and muons, $B \rightarrow D^* m\nu$ in $B \rightarrow D^* e\nu$.

Perhaps the most important result of the Belle II collaboration in 2020 was the method of integrated luminosity measurement [13]. An accurate knowledge of the integrated luminosity (L) is essential since it determines the rate of produced events of a given type through $N = L\,\sigma$ (with σ denoting the cross-section for a particular process). The detec-

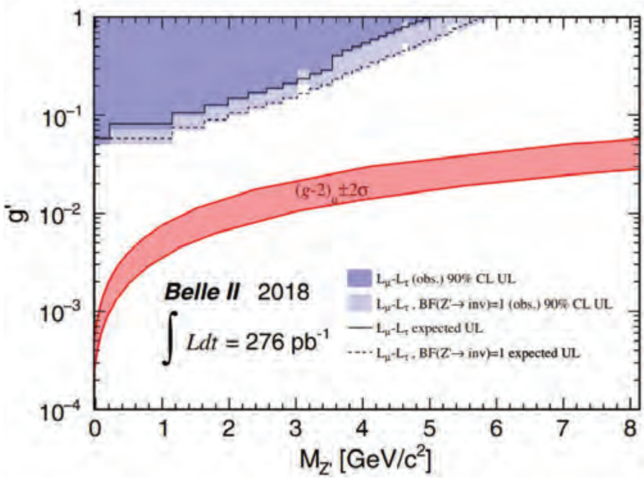

Figure 4: Area in the parametric plane of hypothetical Z' boson mass ($M_{Z'}$) and its coupling constant to muons and τ leptons (g'), excluded at 95% C.L. by the measurement [11]. The red area (not yet experimentally excluded) is the region that could explain the so-called muon anomalous magnetic dipole moment discrepancy.

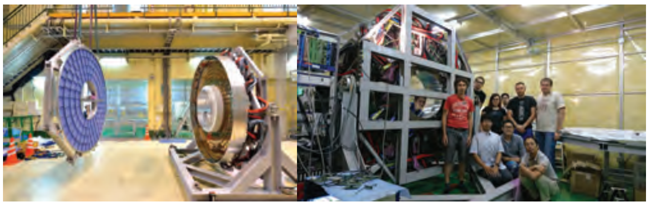

Figure 5: Ring Imaging Cherenkov (RICH) detector with aerogel radiator during assembly. Left: Cherenkov photons emitted by charged particles in a four-centimetre-thick aerogel layer are detected by a large photon detector consisting of 420 hybrid photosensors. Right: Slovenian-Japanese team behind the RICH detector where readout electronics with a multitude of connections can be seen.

tion and reconstruction of processes with accurately known cross-section – in the case of [13] the process is Bhabha scattering and two-photon processes – enables a precise determination of the integrated luminosity.

A European Research Council (ERC) advanced grant was awarded to the project "Flavour Anomalies with advanced particle Identification Methods (FAIME)" lead by prof. Peter Križan, a member of our department. Within this project the decay properties of B mesons into leptons will be measured with high precision. We will try to confirm or refute the preliminary results showing that, under certain conditions, tau leptons behave slightly differentlt to muons and electrons. If confirmed, these results would mean a major revolution in elementary particle physics and in our understanding of nature in general. The crucial component of the Belle II spectrometer for the FAIME project are the charged particle identification detectors (Figure 5). A research group from the JSI, the Faculty of Mathematics and Physics of the University of Ljubljana and the Faculty of Chemistry and Chemical Engineering of the University of Maribor have played a decisive role in their development, preparation and analysis of data taken by these detectors.

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 the 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.

Figure 6: Figure shows one of 1600 ground Cherenkov detectors at the Pierre Auger Observatory. In background communication tower for DAQ data transfer. Detector network covers an area of 3000 km^2.

The Pierre Auger Observatory combines two complementary techniques to measure air showers. On their way through the atmosphere the secondary particles stimulate nitrogen molecules in the air to emit fluorescence light. This light is measured with large telescopes. In addition, secondary particles reaching ground level are registered in an array of particle detectors. The latter are water Cherenkov detectors, measuring the light emitted by relativistic particles passing through a water tank (Figure 6).

The Pierre Auger Collaboration had shown that the energy spectrum of cosmic rays exhibits a sharp drop around 10^{20} eV [14]. 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 the LHC's results, some mysteries were not solved. The number of muons in the 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 Monte Carlo simulations 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 (SSD) are being deployed over the full 3000-km^2 area of the overall surface detector (SD). To enhance the capabilities of the surface detector, especially for composition measurements, it is being equipped with upgraded electronics with a larger sampling rate and a larger dynamic range.

Distributed computing

In 2020, the SiGNET Tier-2 center was running with 8000 CPU cores and 45 PB of storage space. The resources were mostly dedicated to the production and analysis of ATLAS data and Monte-Carlo simulation, and Belle II production. A smaller fraction was used by other departments at the Jožef Stefan Institute and external users in Slovenia. The general purpose NSC cluster at the Jožef Stefan Institute and computing center of ARNES are transparently included in distributed computing infrastructure within WLCG collaboration and EGI infrastructure. HPC.RIVR.UM, a new prototype HPC infrastructure at University of Maribor was added to the grid and supercomputing infrastructure. F9 was participating in EuroHPC activities and contributed to the procurement of Vega EuroHPC supercomputer being built at IZUM in Maribor, which will start operation in March 2021. F9 was also collaborating within the Leonardo consortium, one of the three pre-exascale HPC systems to be procured at Cineca, Bologna. SiGNET-T2 is a full member of international organizations EGI/InSPIRE, wLCG and Nordugrid and participated in several joint projects related to support, maintenance and planning of the computing infrastructure as well as the development, distribution and deployment of the distributed computing infrastructure.

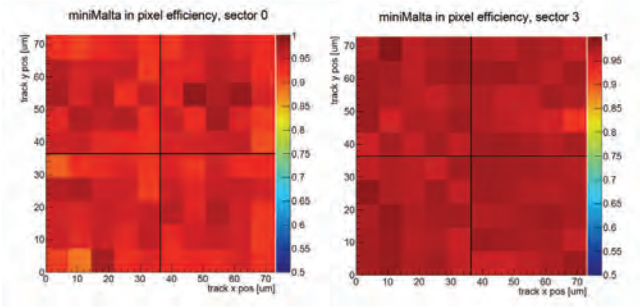

Figure 7: Efficiency of 2×2 pixel detector array on Mini-MALTA chip after irradiation with 1015 n/cm^2 in TRIGA reactor. Figure on the right shows pixel array with modified structure if the low doped n-layer which significantly improves efficiency after irradiation. Measurement was made in the test-beam experiment at ELSA synchrotron in Bonn, Germany (from [15]).

In 2020, SiGNET Tier-2 center was running with 8000 CPU cores and 45 PB of storage space.

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 in the framework of the RD42 collaboration.

Work on an upgrade of the ATLAS detector for the HL-LHC was the main activity in the development of silicon detectors. This includes measurements of silicon strip detectors for ITk 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 2020. Studies were made with test structures on prototype chip RD50-MPW2 developed by the RD50 collaboration. Depleted CMOS is a suitable technology for monolithic tracking detectors for high radiation environments (figure 6) as well as for applications where the amount of material in the tracking volume must be minimized. Depleted CMOS also ensures fast charge collection [15], enabling good time resolution, which is becoming increasingly important in all types of applications.

Our group is working on the development of detectors for next generation of hadron colliders (e.g., Future Circular Collider - FCC). This includes measurements of detector response after irradiation to extreme hadron fluences of 10^{17} n/cm^2 and beyond.

A large number of measurements of space charge concentration as a function of irradiation fluence were made using the E-TCT method [16]. The removal of initial acceptors (boron) caused by neutron irradiation was studied for p-type substrates with different initial resistivities. A study of the behaviour of effective space charge concentration and detector current as a function of annealing time at 60° C was made. A system for E-TCT measurements with active CMOS pixels on an RD50-MPW2 chip was built.

Our group is working on the development of detectors for the next generation of hadron colliders, e.g., Future Circular Collider - FCC. Work includes measurements of the detector's response after irradiation to extreme hadron fluences of 10^{17} n/cm^2 and beyond. In 2020, extensive charge collection measurements with thin planar detectors were made and the results published in [17] (figure 8).

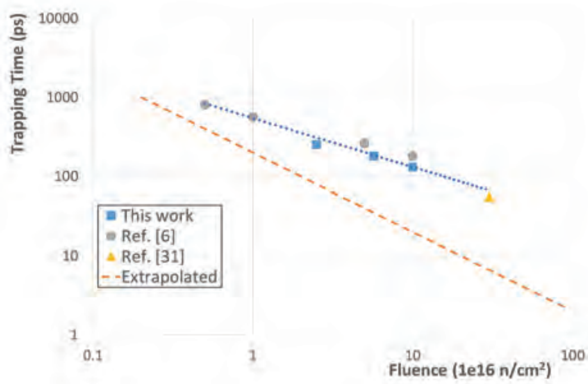

Figure 8: Measurement of effective trapping times in silicon irradiated with neutrons to extreme fluences (from [17]). Measurements show large discrepancies from predictions based on extrapolation of measurements at lower fluences.

Members of the F9 department continued work on diamond detectors for charged particles. Studies of the effects of irradiation with protons and neutrons were made with poly and monocrystalline artificial diamonds [18]. In 2020 measurements of transients caused by two (and more) photon absorption enabling three-dimensional mapping of detector response were made.

As a part of the bilateral project with NürDAM institute, Bolu, Turkey the MOS-FET dosimetry sensors were designed, tested and shown to be appropriate for the use in the ATLAS experiment [19].

Photon detectors

In 2020 we continued with photon sensors' research for a new generation of Cherenkov Ring Detectors (RICH). For the upgrade of the Belle II detector in the forward region 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 will also withstand significant radiation levels, mainly due to neutrons. As a part of this activity, as LHCb collaboration associated technical members, we have established a collaboration with the research groups from the University of Barcelona and Fondazione Bruno Kessler from Trento.

For the upgrade of the Belle II detector in the forward region 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 will also withstand significant radiation levels due to neutrons.

Detectors for medical applications

Experimental particle physics requires the development and mastery of the latest developments in technology. Other fields can benefit from cutting-edge technology we develop in our laboratories. One prolific example is applying to medical physics, where we are introducing advances in photodetectors and readout electronics to improve detection technologies in positron emission tomography (PET) and fluorescence measurements. Leveraging our experience from the design and deployment of Cherenkov detectors in experimental particle physics, we have developed a novel PET detector based on prompt Cherenkov photons detection. In 2020 we produced two multi-channel detector Cherenkov positron emission tomography modules, integrated with fast readout electronics capable of time-of-flight image reconstruction.

The PET detector development is linked with advanced physics simulation and image reconstruction algorithm developments. Our experience has played a central role in proposing a next-generation PET detector exploiting ultra-fast timing and advanced geometries (figure 9). We initiated the collaboration between the University of Barcelona, Fondazione Bruno Kessler, University of California, Davies and Harvard University.

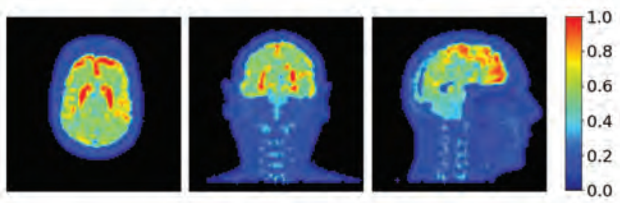

Figure 9: Positron emission tomography is increasingly penetrating the field of medical diagnostics. Using ultra-fast annihilation gamma rays detectors, we can cover only a part of the solid angle. The images obtained with such systems are entirely comparable to the images from the apparatus used today. To design new devices, we use computer simulations with which we can image digital phantoms. The figure shows the reconstructed metabolic activity in the human head in three projections, which is obtained using such an ultra-fast tomograph with a limited field of view.

Detector technologies are also critical in the application of fluorescence lifetime measurements. In 2020 we successfully concluded the EU ATTRACT project, producing a prototype of an ultra-fast fluorescence lifetime acquisition system. The development has attracted the first potential users in biology and pharmaceutical production and received the Jožef Stefan Institute Center for Technology Transfer and Innovation Foundation grant to progress the system's technology readiness level.

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We are also collaborating with CSIC/IFIC, Valencia Spain and the Ohio State University at Columbus, OH, USA in the development of high-resolution detectors and their applications in PET under partial sponsorship of a bilateral Slovenia/USA project. This is a continuous effort of bridging the gap between high-sensitivity detectors found in standard PET rings and sub-millimeter detection probes and combining them to simultaneously achieve high spatial resolution in a selected region of interest with the minimum of interference with standard PET operation.

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. The reactor at IJS is the reference neutron irradiation site for the development of silicon detectors and electronics for LHC and other particle-physics experiments.

Some outstanding publications in the past year

[1] G. Aad et al. (ATLAS Collaboration), "Search for magnetic monopoles and stable high-electric charge objects in 13 TeV proton-proton collisions with the ATLAS detector", Phys. Rev. Lett. 124, 031802, (2020).
[2] G. Aad et al. (ATLAS Collaboration), "Measurement of azimuthal anisotropy of muons from charm and bottom hadrons in ppcollisions at $\sqrt{s}$=13 TeV with the ATLAS detector", Phys. Rev. Lett. 124, 082301, (2020).
[3] G. Aad et al. (ATLAS Collaboration), "Search for heavy Higgs bosons decaying into two tau leptons with the ATLAS detector using pp collisions at $\sqrt{s}$=13 TeV", Phys. Rev. Lett. 125, 051801, (2020).

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[5] G. Kramberger et. al, “Annealing effects on operation of thin Low Gain Avalanche Detectors”, JINST Vol.15 , P08017 (2020).
[6] S. Mazza, G. Kramberger et. al, “Properties of FBK UFSDs after neutron and proton irradiation up to 6e15 neq/cm2”, JINST Vol.15 , T04008 (2020).
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[14] A. Aab et al. (The Pierre Auger Collaboration) , “ Features of the Energy Spectrum of Cosmic Rays above 2.5×10^{18} eV Using the Pierre Auger Observatory”, Phys. Rev. Lett. 125, 121106, (2020).
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[16] R. Klanner et al., “Determination of the electric field in highly-irradiated silicon sensors using edge-TCT measurements”. Nucl. Instr. & Meth. A 951 (2020) 162987.
[17] I. Mandić et al., “Measurements with silicon detectors at extreme neutron fluences”, 2020 JINST 15 P11018.
[18] L. Bäni et al. (RD42 collaboration), ”A study of the radiation tolerance of CVD diamond to 70 MeV protons, fast neutrons and 200 MeV pions.” Sensors, Vol 20, 6648 (2020).
[19] G. Kramberger et al, “Development of MOS-FET dosimeters for use in high radiation fields”, Nucl. Instr. & Meth. A 978 (2020) 164283.

Awards and Appointments

1. Prof. Danilo Zavrtanik, Blinc Award for lifetime achievement in physics, Faculty of Mathematics and Physics, University of Ljubljana and Jožef Stefan Institute, Ljubljana
2. Prof. Andrej Filipčič, Prof. Marko Zavrtanik: Zois Award for Outstanding Achievements in Research of Extreme Energy Cosmic Particles, Ljubljana, Slovenia, Committee of the Republic of Slovenia for the Awarding of Prizes and Recognitions for Outstanding Achievements in Scientific Research and Development

Organization of Conferences, Congresses and Meetings

1. “From visions to reality - proton therapy for cancer treatment in Slovenia”, Jožef Stefan Institute, Ljubljana, Slovenia, 23 January 2020
2. “Researchers’ Night”, Jožef Stefan Institute, Ljubljana, Slovenia, 27 November 2020 (virtual)

INTERNATIONAL PROJECTS

1. COST CA16108 - VBSCan; Vector Boson Scattering Coordination and Action Framework
   Prof. Borut Paul Kerševan
   Cost Office
2. COST VBSCan; Vector Boson Scattering Coordination and Action Framework
   Prof. Borut Paul Kerševan
   Cost Association Aisbl
3. H2020 - AIDA-2020; Advanced European Infrastructures for Detectors at Accelerators
   Prof. Marko Mikuž
   European Commission
4. H2020 - JENNIFER2; Japan and Europe Network for Neutrino and Intensity Frontier Experimental Research 2
   Prof. Rok Pestotnik
   European Commission
5. H2020 - ATTRACT; Real-time Flourescence Lifetime Acquisition System (RfLAS)
   Dr. Rok Dolenec
   European Commission
6. H2020 - FAIME; Flavour Anomalies with advanced particle Identification MEthods
   Prof. Peter Križan
   European Commission
7. Fabrication and Qualification of NürFETs Dosimeters for use at Nuclear Reactors
   Dr. Gregor Kramberger
   Slovenian Research Agency
8. Development of Segmented Silicon and Diamond Radiation Sensors and Readout Electronics for Particle Physics and Medical Diagnostics

Asst. Prof. Igor Mandić
Slovenian Research Agency
9. 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. Marko Mikuž

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. Depleted CMOS Sensors for the ATLAS Tracker Upgrade and Future Collider Experiments
Prof. Marko Mikuž
4. Advanced hadron identification methods for Belle II
Prof. Peter Križan
5. Development of High Granularity Timing Detector for ATLAS experiment
Dr. Gregor Kramberger
6. Resources Review Board
Prof. Marko Mikuž
Ministry of Education, Science and Sport
7. Member of Restricted European Committe for Future Accelerators (RECFA) and Plenary ECFA (PECFA)
Prof. Marko Mikuž
Ministry of Education, Science and Sport
8. Design, Procurement and QA of Flex-rigid Hybrids
Prof. Marko Mikuž
European Organization for Nuclear Research
9. Irradiations in TRIGA Nuclear Reactor
Prof. Vladimir Cindro

VISITOR FROM ABROAD

1. Matthew Franks, University of Liverpool, Great Britain, 9–14 August 2020

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Original Article

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85. Damijan Valentinuzzi *et al.* (12 authors), "[^{18}F]FDG PET immunotherapy radiomics signature (iRADIOMICS) predicts response of non-small-cell lung cancer patients treated with pembrolizumab", *Radiology and oncology*, 2020, **54**, 3, 285-294.
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Review Article

1. AUGER Collaboration, A. Aab *et al.*, "Reconstruction of events recorded with the surface detector of the Pierre Auger Observatory", *Journal of instrumentation*, 2020, **15**, 10, p10021.
2. Paul Lecoq *et al.* (22 authors), "Roadmap toward the 10 ps time-of-flight PET challenge", *Physics in medicine & biology*, 2020, **65**, 21, 21RM01.
3. AUGER Collaboration, A. Aab *et al.*, "The Pierre Auger Observatory and its upgrade", *Science reviews*, 2020, **1**, 4, 8-33.

Published Conference Contribution (invited lecture)

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Published Conference Contribution

1. Rok Pestotnik *et al.* (29 authors), "Front-end electronics of the Belle II aerogel ring imaging detector", In: *RICH 2018, 10th International Workshop on Ring Imaging Cherenkov Detectors, July 29-August 4, 2018, Moscow, Russia*, Proceedings, (Nuclear instruments and methods in physics research A **952**), 2020, 161711.
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9. Rok Pestotnik, "Use of Cherenkov light in TOF-PET", In: *FATA 2019, International workshop Fast Timing Applications for Nuclear Physics and Medical Imaging, 3-5 September, 2019, Acireale, Spain*, Proceedings, (Il Nuovo cimento C **43** 1), 18.
10. Rok Pestotnik, Rok Dolenec, Andrej Seljak, Matej Mrak, "Real-time fluorescence lifetime acquisition system", In: *13. ITTC, 13th International Technology Transfer Conference, 8 October 2020, Ljubljana, Slovenia*, Proceedings of the 23rd International Multiconference Information Society (IS 2020), volume E, Institut "Jožef Stefan", 2020, 33-37.
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THESES AND MENTORING

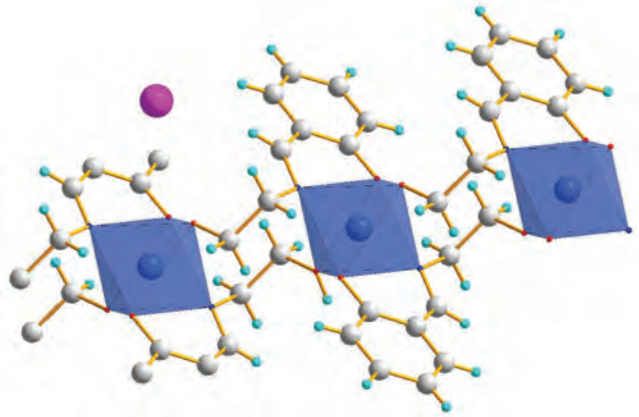
1. Bojan Hiti, *Radiation hardness of CMOS detector prototypes for ATLAS Phase-II ITk upgrade:* doctoral dissertation, Ljubljana, 2020 (mentor Igor Mandić).
2. Tadej Novak, *Search for type-III seesaw heavy leptons with the ATLAS detector at the LHC:* doctoral dissertation, Ljubljana, 2020 (mentor Borut Paul Kerševan).

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 elements of the main groups, the synthesis of new hybrid materials and inorganic materials with special properties. A large part of the group's activity is devoted to technological, environmental and process-safety issues in Slovenia. The group has been working closely with Slovenian industry for more than 30 years. It is also active in the field of education and in promoting science among students at universities and primary schools.

Head:
Asst. Prof. Gašper Tavčar

By treating gaseous, liquid or solid fluorides with UV-photolyzed O_2/F_2 mixtures and by treating solid oxides with UV-photolyzed F_2 (or O_2/F_2 mixtures) in liquid anhydrous HF at room temperature, we investigated the possibility of preparing $O_2M^{III}F_4$ (M = B, Fe, Co, Ag), $O_2M^{IV}F_5$ (M = Ti, Sn, Pb), $(O_2)_2M^{IV}F_6$ (M = Ti, Ge, Sn, Pb, Pd, Ni, Mn), $O_2M^{IV}{}_2F_9$ (M = Sn), $O_2M^{V}F_6$ (M = As, Sb, Au, Pt), $O_2M^{V}{}_2F_{11}$ (M = Pt), $O_2M^{VI}F_7$ (M = Se), $(O_2)_2M^{VI}F_8$ (M = Mo, W), and $O_2M^{VII}F_8$ (M = I). The approach was successful in the case of the previously reported O_2BF_4, O_2MF_6 (M = As, Sb, Au; Pt), O_2GeF_5, and $(O_2)_2(Ti_7F_{30})$. Novel compounds $O_2GeF_5{\cdot}HF$, α-$O_2Sn_2F_9$ (1-D) and the HF - solvated and non-solvated forms of β-$O_2Sn_2F_9$ (2-D) were synthesized and their crystal structures were determined by single-crystal X-ray diffraction. The anionic parts of the crystal structures of all these materials arise from the condensation of octahedral MF_6 (M = Ge, Sn) units. The anion in the crystal structure of $O_2GeF_5{\cdot}HF$ consists of infinite $([GeF_5]^-)_\infty$-chains of GeF_6 octahedra sharing common vertices. The crystal structure of α-O_2SnF_9 (1-D) is composed of polymeric $([Sn_2F_9]^-)_\infty$ anions that appear as two parallel infinite chains of SnF_6 units, where each SnF_6 unit of one chain is connected to a SnF_6 unit of the second chain via a common fluorine vertex. A single-crystal structure determination of $[O_2][Sn_2F_9]{\cdot}0.9HF$ shows that it consists of two-dimensional $([Sn_2F_9]^-)_\infty$. The 2D grids have a wave-like conformation. The $([Sn_2F_9]^-)_\infty$ layer contains both six- and seven-coordinated Sn(IV) atoms that are interconnected by bridging fluorine atoms. A new, more complex $[O_2]^+$ salt, $O_2[Hg(HF)]_4[SbF_6]_9$, has also been prepared. In its crystal structure, the Hg atoms bridge to SbF_6 units to form a 3D framework. Attempts to prepare several chlorine analogs of O_2^+ fluorine salts (i.e., O_2TiCl_5 and O_2MCl_6 (M = Nb, Sb)) failed.



Fragment of the crystal structure with $C_{18}H_{20}N_2O_4IMn$ composition, published in Cryst. Growth Des. 2020, 20, 1491–1502

By a direct synthesis method, oxidative dissolution of manganese powder in the presence of Schiff bases, ammonium salt and oxygen in air, we have prepared a family of eight polymeric manganese complexes (III). According to the results of an X-ray structural analysis, the main structural feature of the compounds is the one-dimensional polymer structure. In most cases, the cationic chains and anions are connected by electrostatic interactions and hydrogen bonds. However, in one case, the polymers are composed of neutral units. The compounds were also characterized by electronic paramagnetic resonance. The study was also complemented by ab-initio CASSCF and DFT calculations. The research was carried out in collaboration with research groups from the Ukraine, France and the USA.

Asst. Prof. Matic Lozinšek was awarded an ERC Starting Grant worth €2.37 million

Associate of the Jožef Stefan Institute, Asst. Prof. Dr. Matic Lozinšek, was the only Slovene to succeed in obtaining a 5-year project in a tender of the European Research Council for researchers starting an independent research career. ERC Starting Grant, European Research Council, "Challenging the Oxidation-State Limitations of the Periodic Table via High-Pressure Fluorine Chemistry - HiPeR-F", 2021–2026. The HiPeR-F project focuses on the study of chemical reactions with fluorine under extremely high pressures – from 10,000 bar to over 100,000 bar. The element fluorine, which can be called the tiger of the periodic table, due to its extraordinary reactivity, will enable the testing of the limits of chemistry under extreme conditions. The project is thus a combination of two specialized experimental as well as extreme research

European Research Council
Established by the European Commission

Figure 2: ERC Starting Grant – HiPeR-F, study of chemical reactions with fluorine under extremely high pressure

Research in the field of technological solutions for better use of secondary sources of raw materials

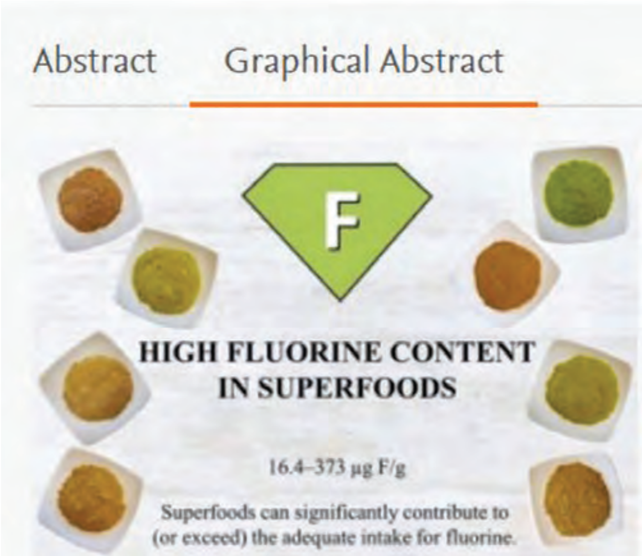


Figure 3: JFC abstract – High fluorine content in superfoods, published in Journal of Fluorine Chemistry, 2020, vol. 234

areas – the study of substances under extremely high pressures and the study of extreme chemical reactivity. It is expected that if the experimental barriers and difficulties in dealing with the most reactive halogen under high pressure can be overcome, this will lead to discoveries that will influence and broaden our understanding of the periodic table of elements.

We determined the total fluoride content in some types of plant superfoods. In eight of the fifteen cases (16-373 µg/g), it was significantly higher than the fluorine content in plants from uncontaminated areas (10 µg/g). Consumption of such foods might contribute significantly to the daily intake of fluoride, which can thus exceed an appropriate daily intake.

We participated in a study on the influence of the anodization electrolyte aging on its composition. It was shown that batch-type anodization cells cannot yield reproducible TiO_2 nanotube films due to the aging of the anodization electrolyte and that continuous regeneration of the anodization electrolyte is necessary to obtain TiO_2 films with comparable photocatalytic activities.

We continued writing review articles for Structural Chemistry journal; a short summary of each article, a thermochemical comment and suggestions for future research are added.

As part of the renovation of the analytical laboratory, the laboratory was equipped with an instrument for atomic emission spectrometry with inductively coupled plasma and a system for the microwave digestion of samples.

In accordance with the principles of the circular economy, we started research on the use of secondary resources - the reprocessing of waste slag from the recycling of lead-acid batteries. Despite an efficient recycling process, the slag still contains significant amounts of lead, which remain in it along with other useful materials. Together with other research groups, we are trying to separate and reuse lead, iron and anthracite from the waste slag.

Within the topic of process safety, in 2020 we researched and published work on the introduction of the safe use of Liquefied Natural gas (LNG) for ships propulsion (European project SUPER-LNG), the connection between leadership styles and safety management systems in industrial organizations, and the resilience and protection of sensitive industrial sites and facilities (critical infrastructure) against physical, cybernetic, technological hazards and extreme natural phenomena (European project InfraStress). In addition, we were researching safety challenges in industrial organizations related to the outbreak COVID-19 pandemic. We started working 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).

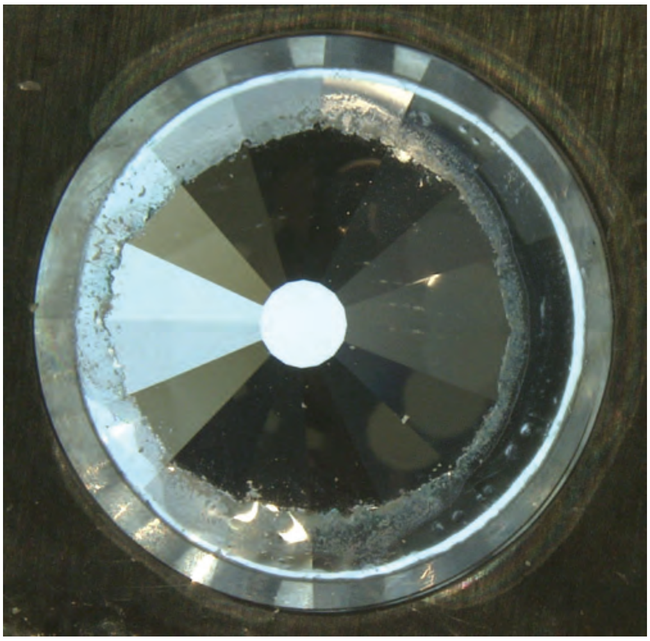


Figure 4: Diamond anvil for the study of matter under high pressure

We continued with our activities in the field of education and the promotion of science. Members of the department actively participated in the work of the Jožef Stefan International Postgraduate School as lecturers and as mentors for M.Sc. and Ph.D. students. In addition, the School of Experimental Chemistry maintained its very important relations with primary and secondary schools and even kindergartens through experimental courses conducted in a specialized laboratory or through direct demonstrations in schools. With demonstrations of chemical experiments, this year mainly with on-line demonstrations, we participated in the festival Play with me and the Slovenian Science Festival. Nevertheless, we were also able to carry out some activities of the School of Experimental Chemistry with the direct participation of students. Some of the activities of the School of Experimental Chemistry were carried out within the project funded by JSI and the City of Ljubljana.

The promotion of science, research and non-formal education is also linked to the European Action Researchers' Night under the Horizon 2020 programme. At the end of November 2020, we organized and carried out a series of activities as part of this project, which were moved online due to the COVID-19 epidemic. Despite the circumstances, we believe that the objectives of the project were achieved.

Some outstanding publications in the past year

1. D. Kurzydłowski, S. Kobyakov, Z. Mazej, S. B. Pillai, B. Chakraborty, P.K Jha, Unexpected persistence of cis-bridged chains in compressed AuF_3, *Chemical Communications*, 2020, vol. 56, no. 36, page 4902-4905.
2. Z. Mazej, E. A. Goreshnik, X-ray crystal structures of α- and β-$O_2Sn_2F_9$, $O_2Sn_2F_9$·0.9HF, O_2GeF_5·HF, and $O_2[Hg(HF)]_4(SbF_6)_9$. *Inorganic Chemistry*, 2020, vol. 59, no. 3, page 2092-2103.

Organization of conferences, congresses and meetings

1. Matic Lozinšek, member of organizing committee, Slovenian Chemistry Days 2020, 16.–18. 9. 2020, Portorož, Slovenia
2. Melita Tramšek, Researchers' night 2020 on "Jožef Stefan" institute, 27. 11. 2020, Ljubljana, Slovenia

Patent granted

1. Tomasz Gilewski, Piotr Połczyński, Jakub Gawraczyński, Rafał Jurczakowski, Piotr J. Leszczyński, Wojciech Grochala, Zoran Mazej, Silver (II) sulfate (VI) hydrate and method to synthesize it, PL234672 (B1), Urząd Patentowy Rzeczypospolitej Polskie, 31. 03. 2020.
2. O. Stetsiuk, N. Plyuta, N. Avarvari, E. A. Goreshnik, V.N. Kokozay, S. R. Petrušenko, A. Ozarowski, Mn(III) chain coordination polymers assembled by salicylidene-2-ethanolamine schiff base ligands: synthesis, crystal structures, and HFEPR study. *Crystal Growth & Design*, 2020, vol. 20, no. 3, page 1491-1502.
3. Z. Mazej, Noble-gas chemistry more than half a century after the first report of the noble-gas compound. *Molecules*, 2020, vol. 25, no. 13, page 3014-1-3014-18.
4. D. Štepec, G. Tavčar, M. Ponikvar-Svet, Surprisingly high fluorine content in some exotic superfoods. *Journal of Fluorine Chemistry*, 2020, vol. 234, page 109521-1-109521-6.

INTERNATIONAL PROJECTS

1. 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
2. H2020 - NOCMOC; European Researchers' Night (NIGHT)
   Dr. Melita Tramšek
   European Commission
3. 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. The quest for high-temperature superconductvity and exotic magnetism in fluoridoargentates(II)
   Asst. Prof. Matic Lozinšek
2. Utilization of secondary lead slag as a secondary raw material for the production of lead
   Asst. Prof. Gašper Tavčar
3. Evaluation of greenhouse gasses mitigation measures in industry
   Dr. Robert Kocjančič
4. SUstainability PERformance of LNG-basedmaritime mobility
   Prof. Marko Gerbec
   The Emillia-romagna Region
5. Innovative ECO plasma seed treatment (for sowing and for human and animal diet/nutrition
   Asst. Prof. Gašper Tavčar
   Ministry of Education, Science and Sport
6. Evaluation of greenhouse gasses mitigation measures in industry
   Dr. Robert Kocjančič
   Ministry of the Environment and Spatial Planning

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. Prof. dr Simon Parsons; School of Chemistry and Centre for Science at Extreme Conditions, The University of Edinburgh, Edinburgh, United Kingdom, 4.2.2020 to 7.2.2020

STAFF

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

Postgraduates
10. Jan Gnidovec, B. Sc.

11. Evelin Gruden, B. Sc.
12. David Levovnik, B. Sc.
13. *Dona Štepec, B. Sc., left 01.05.20*
14. *Žiga Zupanek, B. Sc., left 01.05.20*

Technical officers

15. Tine Oblak, M. Sc.
16. Tomaž Ogrin, M. Sc.

Technical and administrative staff

17. Peter Frkal, B. Sc.
18. Pero Kolobarić
19. Robert Moravec
20. Mira Zupančič

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Original Article

1. Andrii A. Fedorchuk, Evgeny A. Goreshnik, Yurii Slyvka, Marian G. Mys'kiv, "Cu(I) arylsulfonate π-complexes with 3-allyl-2-thiohydantoin: the role of the weak interactions in structural organization", *Acta chimica slovenica*, 2020, **67**, 4, 1148-1154.
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1. Dona Štepec, *Determination of fluorine in some food and environmental samples:* doctoral dissertation, Ljubljana, 2020 (mentor Maja Ponikvar-Svet).
2. Žiga Zupanek, *Reactions of fifth group Lewis acids with nitriles and imidazolium-based compounds:* doctoral dissertation, Ljubljana, 2020 (mentor Gašper Tavčar).

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, as well as the synthesis of new compounds. The synergy of these fields is created in the studies of corrosion protection and functionalization 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 density functional theory (DFT) methods.

Head:
Prof. Ingrid Milošev

Corrosion is a widespread phenomenon with enormous economic and environmental impact. The cost of corrosion damage is estimated at € 2.5 trillion per year worldwide. Due to these huge costs, the protection of metals and alloys is essential. Corrosion protection with the main goal to prolong the lifetime of metal materials is one of the important methodologies to reduce the need for steeply increasing production and thus preserve resources for future centuries. 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 the development of 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 – corrosion inhibitors, conversion coatings, organic coatings and inorganic coatings (Figure 1) – for major metal and alloy groups, which are indispensable in today's era, 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 to reduce emissions into the environment. Steels and alloys based on copper are indispensable materials in the field of infrastructure, construction, etc.

The type of anchor group of an organic corrosion inhibitor is crucial for adsorption on Al. Among the investigated anchor groups, the phosphonic group forms stable adsorbed layers, while the carboxylic group does so only for long alkyl chains. Other anchor groups do not show noticeable adsorption affinity and the corresponding compounds are inefficient for inhibiting the corrosion of Al.

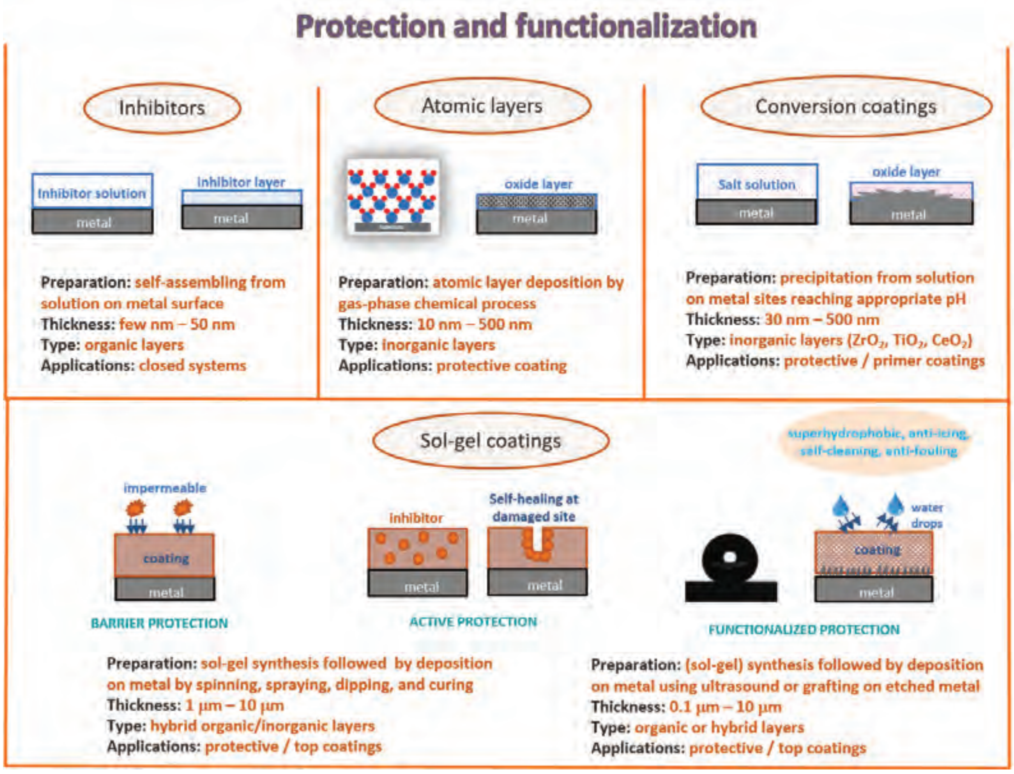

Figure 1: Types of corrosion protection and functionalization of materials.

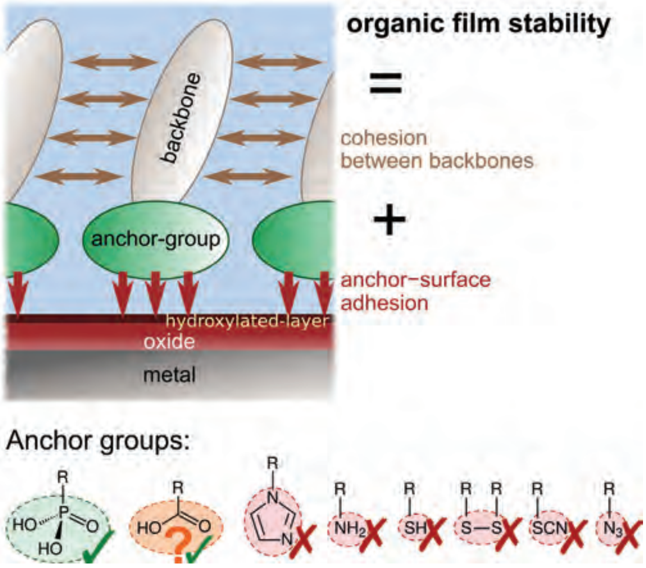

Figure 2: Archetypal structure of investigated organic surfactant inhibitors consist of reactive anchor group and alkyl backbone. The stability of the adsorbed organic layer depends on the anchor-group–surface adhesion and lateral cohesion between the backbones. Among the investigated anchor groups, the phosphonic group forms inhibitive adsorbed layers on the Al surface, irrespective of the alkyl chain length, while the carboxylic group can form such layers only for long alkyl chains. Other anchor groups do not show noticeable adsorption affinity and the corresponding compounds are inefficient for inhibiting the corrosion of Al.

Even something as conceptually simple as the adsorption of electronegative atoms on metal surfaces, where repulsive lateral interactions are expected for obvious reasons, can lead to unanticipated behaviour, such as apparent attractive interactions between adsorbed anions.

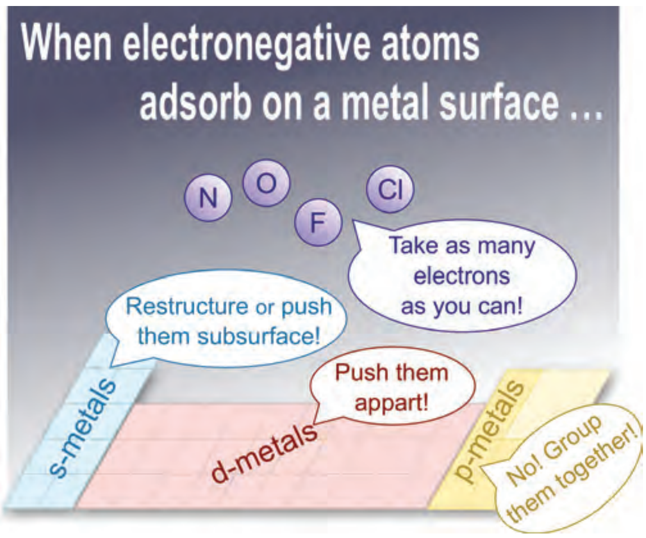

Figure 3: Schematically indicated predominant scenarios for lateral interactions between adsorbed electronegative atoms on the metal surfaces. On s-metals, negative atoms either induce surface restructuring or penetrate below the surface. On d-metals the lateral interactions between adatoms are repulsive, whereas on p-metals the lateral interactions between the electronegative adatoms can be surprisingly attractive.

In our laboratory we investigate all of the above-mentioned alternatives (Figure 1) and even combine them with each other, e.g., sol-gel coatings and inhibitors in order to achieve not only barrier protection, but also active protection, where the coating after corrosion damage is able to self-heal. We also introduce modern methodologies, such as atomic layer deposition (ALD), in corrosion protection.

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

Integrative experimental–modelling approach

In-depth fundamental knowledge of surface processes is needed to design effective corrosion protection, because 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 or organic synthesis, (2) electrochemical and surface analysis techniques, and (3) modelling and simulations based on first-principles DFT. In this context, we investigated alkyl-based organic compounds as surfactant corrosion inhibitors, whose molecular structures consist of a reactive anchor group and an alkyl backbone. We addressed the effect of the anchor group and alkyl backbone chain on the performance of organic compounds as corrosion inhibitors for aluminium using an integrative experimental–modelling approach. Nine different anchor groups (azide, imidazole, thiocyanate, amino, disulfide, thiol, phosphonic, carboxyl, and benzoic) and two different alkyl backbones (octyl and octadecyl) were investigated. Our study clearly demonstrated that the corrosion resistant and superhydrophobic properties depend on the anchor group, which governs adhesion to the surface, and backbone, which is responsible for lateral cohesive interactions (Figure 2). The morphology and chemical composition of modified layers were studied using scanning electron microscopy, X-ray photoelectron spectroscopy and time-of-flight secondary-ion mass spectrometry. Electrochemical and long-term immersion properties were investigated in 0.5 M NaCl. Calculations based on DFT were performed to model the adsorption of selected anchor groups on the hydroxylated oxidized aluminium surface. Integrated results allowed the identification of the anchor groups that are able to form inhibitive adsorbed layers on Al surface regardless of the alkyl chain length (phosphonic acids), those that are able to form such layers only for long alkyl chain length (carboxylic acids), and those that are not able to form adsorbed layers at all and are thus not efficient corrosion inhibitors.

Further attention was then given to *n*-alkyl carboxylic acids (CA), which can form inhibitive adsorbed layers only when the carboxylic head-group is attached to the long alkyl backbone. In particular, with DFT-based molecular modelling we systematically addressed the roles of adsorption mode, molecular coverage, alkyl chain tilt-angle, and alkyl chain length on the stability of the formed CA monolayers. The adsorption was modelled on two models of the hydroxylated ultrathin-oxide film supported on aluminium. We considered plain adsorption and adsorption via the condensation mechanism. While on a fully hydroxylated surface only the monodentate carboxylate bonding mode was identified, the bidentate mode was found to be viable near OH vacancies. We showed that the adsorption energy can be decomposed into two components: (i) the anchor-group–surface adhesion and lateral cohesion between alkyl backbones. While the anchor-group–surface interaction is largely independent of the alkyl chain length, lateral intermolecular interactions are proportional to the number of C atoms in the alkyl chain. Consequently, adsorption is stabilized by about 1 eV/molecule at full monolayer coverage when the alkyl chain length increases from 2 to 18 C atoms.

In the context of the initial stages of the oxidation and passivation of metal surfaces, we systematically investigated, by means of DFT calculations, the adsorption of four different electronegative atoms on 70 surfaces of 44 elemental metals and showed that even something as conceptually simple as the adsorption of electronegative atoms on metal surfaces, where repulsive lateral interactions are expected for obvious reasons, can lead to unanticipated behaviour, such as apparent attractive interactions between adsorbed anions. With the aid of a simple developed model, we explained the origin of the surprising lateral interactions between electronegative adatoms observed on some metal surfaces. Four different scenarios for lateral interactions were identified, some of them being unexpected (Figure 3): (i) They are repulsive, which is the typical case and occurs on almost all the transition metals. (ii, iii) They are atypical, being either attractive or negligible, which occurs on p-block metals and Mg. (iv) Surface restructuring stabilizes the low-coverage configuration, preventing atypical lateral interactions. The last case occurs predominantly on s-block metals.

Corrosion protection and functionalization of materials

Conversion coatings can be defined as coatings formed by conversion from soluble salt to a slightly soluble or insoluble oxide and/or hydroxide that precipitates either throughout the metal surface or at intermetallic particles that are electrochemically more noble with respect to the surrounding matrix and where oxygen reduction takes place. Conversion coatings based on the salts of rare earths, zirconium or titanium are an important research direction in the search for novel corrosion protection. Cerium- and lanthanum rare-earth conversion coatings were deposited from solutions of $CeCl_3$ and $LaCl_3$ salts on three aluminium-based substrates, i.e., Al, AA2024-T3 and AA7075-T6, to investigate the effect of conversion temperature, conversion time and the addition of hydrogen peroxide. Coatings prepared under different conditions were then analysed in terms of corrosion properties in 0.1 M NaCl, morphology, topography and composition. Morphology and composition of the coatings were analysed using scanning electron microscopy with energy-dispersive X-ray spectroscopy and X-ray photoelectron spectroscopy. Representative SEM images are given for La-based coatings in Figures 4a-c. The corrosion resistance, morphology, composition and homogeneity of coatings were largely dependent on the parameters of the conversion treatment and the type of substrates. The most corrosion resistant were the Ce-based coatings produced at 60 °C for 1 h in a bath containing $CeCl_3$ and H_2O_2. The La-based coating did not reach a comparative resistance when deposited under the same conditions. The morphology of the coatings ranged between individual deposits to thick, cracked coatings with a nodular morphology. Ce-based coatings predominantly contained Ce(IV) hydroxide when formed with added H_2O_2. La-based coatings contained La(III) hydroxide mixed with Al(III) hydroxide.

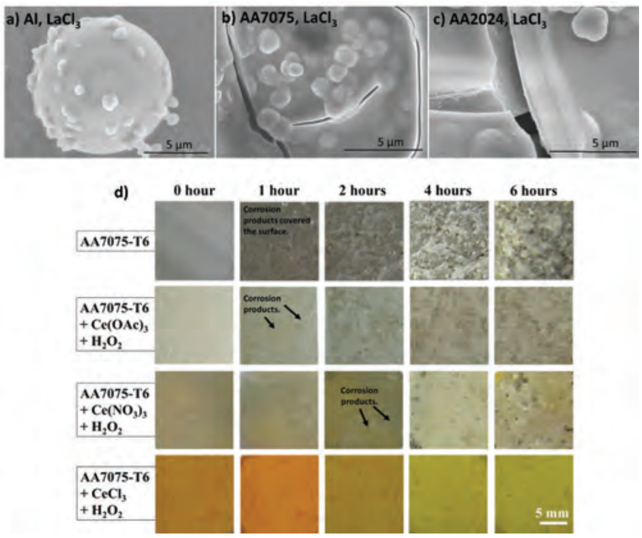

Figure 4: SEM images recorded at (a) aluminium, (b) aluminium alloy 7075, and (c) aluminium alloy 2024 substrates coated with conversion coatings formed in a conversion bath of 0.01 M $LaCl_3$ and 0.13 M H_2O_2 for 1 h at 60 °C. (d) Images of AA7075 samples coated with Ce-based conversion coatings after exposure to salt-spray chamber.

Cerium conversion coatings were also formed in a conversion bath of 0.05 M cerium salt and 0.25 M hydrogen peroxide at room temperature. Various cerium salts were used: Ce(III) acetate, Ce(III) nitrate and Ce(III) chloride (Figure 4d). The conversion process from Ce^{3+} to Ce^{4+} was followed by UV-vis spectroscopy. The conversion of cerium coatings on the alloy surface was monitored by measuring the open-circuit potential. To investigate the corrosion properties of uncoated and coated samples, the linear polarization and electrochemical potentiodynamic curves were recorded in 0.1 M NaCl. Additionally, salt-spray-chamber testing was carried out. Samples were characterized by scanning electron microscopy. Results revealed that the cerium conversion and corrosion resistance were dependent on the type of cerium salt and conversion time in the conversion bath. The most compact and uniform cerium conversion coating were produced from solution of cerium(III) acetate, but better protection was obtained in nitrate and, especially, chloride solutions due to thicker coatings (Figure 4d). Selected cerium conversion coatings showed the ability to

Zirconium conversion coatings offer good corrosion protection when deposited on aluminium alloys and even show the ability to self-seal; however, the degree of protection is dependent on the type of alloy.

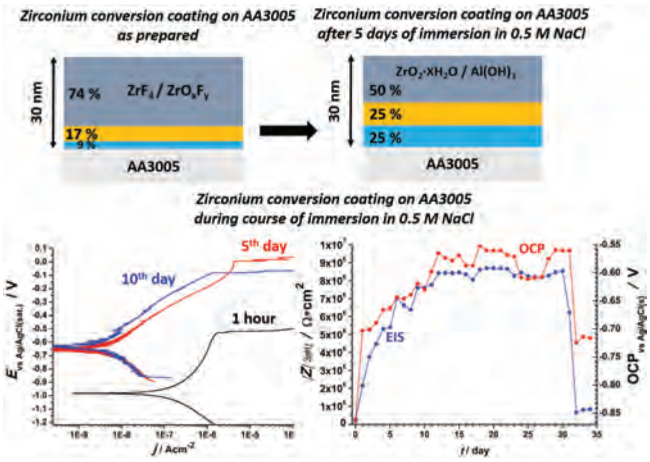

Figure 5: Schematic presentation of the structure of Zr conversion coating deposited on aluminium alloy AA3005 before and after immersion in 0.5 M NaCl (upper panel). The coating shows a self-sealing ability due to densification related to the leaching of fluoride and the formation of Al(III) hydroxide. Potentiodynamic polarization curves and (left) and impedance and open-circuit potential (right) are given as a function of immersion time in 0.5 M NaCl. (lower panel).

protect AA7075-T6 under moderate, non-rigorous corrosive conditions. Coatings are relatively easy to prepare, are low-cost and non-toxic.

Zirconium conversion coatings (ZrCCs) were prepared on aluminium-manganese alloy AA3005 by immersion in 200 ppm of H_2ZrF_6 bath for 10 minutes at room temperature. Potentiodynamic polarization curves and electrochemical impedance spectra were measured up to 10 and 40 days, respectively, in 0.5 M NaCl solutions. Microstructural characterization of the samples was carried out using scanning electron microscopy equipped with energy-dispersive X-ray spectroscopy, X-ray photoelectron spectroscopy, time-of-flight secondary-ion mass spectrometry, focused-ion-beam microscopy and transmission electron microscopy. The coating had a tri-layer structure with a thickness of 200 nm in the proximity of intermetallic particles and 30 nm far from intermetallic particles at the coating matrix (Figure 5). After immersion of 5 days in 0.5 M NaCl solution, the overall thickness of the coating did not change, but the proportion of the individual layer changed, as well as the microstructure and composition, i.e., a transformation of ZrF_4/ZrO_xF_y to $ZrO_2 \cdot 1.2H_2O_{(s)}$ and the formation of $Al(OH)_3$ in the top layer of ZrCC, respectively. Mn segregated in the bottom layer of ZrCC. The thickness of the top layer decreased and that of the middle, and especially, the bottom layer increased. Upon immersion in NaCl, a hat consisting mainly of ZrO_2 with a small amount of Al formed above and around (Mn, Fe) IMPs. However, at prolonged immersion channels around IMPs became filled with a dense layer of aluminium oxide leading to passivation. At the same time, the concentration of fluorine decreased, while that of O increased, especially in the middle and bottom layers of the ZrCC. Electrochemical measurements showed that the corrosion resistance of the ZrCC on AA3005 were improving during immersion in the NaCl solution, i.e., impedance value at low frequency increased with immersion time, reaching an average value of $8.5 \cdot 10^6\ \Omega \cdot cm^2$ at 3 mHz after 10 days of immersion. These results indicate that ZrCC on AA3005 alloy exhibits a self-sealing/active corrosion protection behaviour during immersion in a 0.5 M NaCl solution. Its corrosion performance seems to be equal or better than that usually observed for chromium conversion coatings. It was proposed that Mn from AA3005 together with Zr from ZrCC are able to trigger a self-sealing and active corrosion protection within the coating by incorporation in the bottom part of the conversion coating. These are very promising results, and we suggest that future formulas of ZrCC should include Mn.

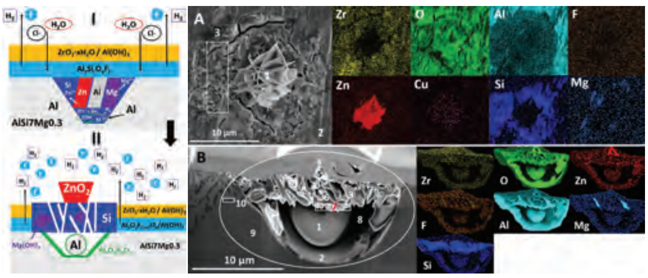

Figure 6: (left panel) Schematic presentation of the self-sealing mechanism of zirconium conversion coating applied on AlSi7Mg0.3 alloy during its immersion in 0.5 M NaCl. (right panel) (a) Top view and (b) side view SEM images with EDS mapping (right) of a cross-section of ZrCC-200 on AlSi7Mg0.3 prepared for a conversion time of 10 minutes after 5 days of immersion in 0.5 M NaCl solution.

The mechanism of formation of ZrCCs was studied on other aluminium alloys as well. For AlSi7Mg0.3 alloy, the electrochemical characterization demonstrated the improvement of the corrosion resistance of AlSi7Mg0.3 during the first 4 days of immersion in 0.5 M NaCl. This is followed by the occurrence of pitting, as reflected in a drop of impedance modulus at 3 mHz. However, on longer immersion, the value of $|Z_{3mHz}|$ recovered up to $1.5 \cdot 10^6\ \Omega \cdot cm^2$ and remained at that value until the end of the immersion. This electrochemical behaviour suggests that active corrosion protection takes place for ZrCC applied on AlSi7Mg0.3. The following mechanism of self-sealing/active corrosion protection in ZrCC applied to AlSi7Mg0.3 (Figure 6): Electrolyte penetrates into ZrCC through defects down to IMPs and Si-crystallites, where the corrosion process initiated. In these areas, evolution of H_2 takes place and alkalinity increases. Weak spots under ZrCCs were Zn-rich. We assume that the spots may be Al-Mg-Zn intermetallic particles (IMPs); at these spots the corrosion process was intense and led to de-alloying of the Zn, Mg and Al. This process caused the cracking of ZrCCs at the surface. However, Zr and Si were apparently able to migrate to the pit walls and become incorporated into the dense conversion layer consisting mainly of aluminium oxide. This leads to the conclusion that Si and Zr may play a role in stabilizing the aluminium oxide and preventing its dissolution. The majority of the ZrCC coating was not subjected to pitting because of the self-sealing of ZrCCs. OH^- ions and H_2(g) moved towards the outer interface with electrolyte, causing leaching of F^- ions from the coating. This causes the transformation of ZrF_4/ZrO_xF_y into $ZrO_2 \cdot xH_2O_{(s)}$. In the electrolyte, F^- ions are equilibrated with Na^+ ions. ToF-SIMS analysis showed that F^- ions could be exchanged with Cl^- ions and incorporated into the coating structure. We believe that, simultaneously with the hydrogen evolution reaction, dissolution of Si/SiO_2 in the presence of F^- ions could take place at a low pH inside the pit; Si could be dissolved from Si-crystallites and/or

IMPs and play a role in improving the corrosion resistance of ZrCCs by the formation of $SiO_2 \cdot 2H_2O$ during the first 4 days of immersion in 0.5 M NaCl.

Zirconium conversion coatings prepared in a 200-ppm H_2ZrF_6 bath for optimal conversion times, were applied on aluminium alloys starting from AA1xxx up to AA7xxx series. The electrochemical behaviour and self-sealing abilities of the coatings were studied by electrochemical impedance spectroscopy during their immersion in 0.5 M NaCl for five days. All the zirconium conversion coatings had a bi-layer structure, with an average thickness in the range 30–60 nm, except for the coating applied on alloy AA2024, which exhibited a single-layer structure with a thickness of 12 nm. The coatings provided excellent corrosion protection and self-sealing behaviour when applied on AA3005, AAA356.0, and very good corrosion protection for AA380.0, AA5754 and AA1050A. On the other hand, these coatings did not provide adequate corrosion protection for AA2024 and AA7075. The results were discussed in terms of the role of intermetallic particles on the properties of the conversion coating. The main reason for the corrosion protection of ZrCC-7075 being poor was that the content of Zn in the matrix was too high (5.81 wt.%). Even for ZrCC-A356.0 and ZrCC-380.0, which contain substantially lower contents of Zn in the matrix (0.07 and 1.2 wt.%, respectively), the pitting was initiated at Zn-rich areas. Proper surface pre-treatment for AA7075 before applying ZrCC could improve the performance of ZrCC significantly. Optimal pre-treatment for AA7075 should remove or passivate Zn-rich IMPs at the alloy surface before the application of ZrCC.

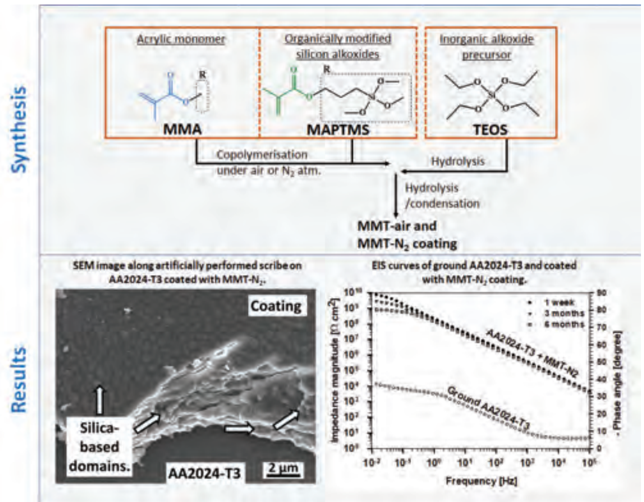

Figure 7: Synthesis and characterization of acrylate-based hybrid sol-gel coating for the corrosion protection of the aluminium alloy AA2024.

A very important part of our research comprises various hybrid sol-gel coatings designed to protect aluminium alloys or steel in a chloride environment. We are currently investigating several types of coatings in our laboratory. Polysiloxane coatings MMT is an acrylate-based coating combining 3-methacryloxypropyl trimethoxysilane (MAPTMS) copolymerized with methyl methacrylate (MMA), and hydrolysed tetraethyl orthosilicate (TEOS) (Figure 7). We studied the optimisation of the copolymerisation process of acrylate-based hybrid sol-gel coating to obtain long-lasting corrosion protection of AA2024-T3. The sol synthesis was evaluated at various stages using *real-time* Fourier transform infrared spectroscopy (FTIR), multinuclear liquid- and solid-state magnetic resonance spectroscopy and gel-permeation chromatography. After deposition on AA2024-T3 substrate and curing, the coating properties were further evaluated by contact profilometer and focused-ion-beam/scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy. The corrosion performance was evaluated in 0.1 M NaCl solution using electrochemical impedance spectroscopy and salt-spray-chamber testing. The results indicated that the reaction performed in the nitrogen atmosphere increases the degree of copolymerisation of acrylates groups, resulting in a larger molecular weight of the formed copolymer. After curing, both sol-gels formed continuous, smooth, ~4-µm-thick coatings that provided excellent barrier properties. However, when the coating was synthesised under a nitrogen atmosphere, the coating provided better long-term corrosion resistance, reaching almost 1 GΩ cm^2 after 6 months of immersion in a 0.1 M NaCl solution. Superior corrosion resistance was also confirmed in the salt-spray chamber where the coating prepared under a N_2 atmosphere remained unchanged for more than 500 hours.

The properties of polysiloxane-acrylate-based coatings can be improved by the optimisation of co-polymerization parameters, i.e. time and proper choice of gas atmosphere, between and methyl methacrylate (MMA) and 3-methacryloxy-propyl trimethoxysilane (MAPTMS).

In addition to copolymerization atmospheres, the effect of copolymerization time was also studied. The reactions taking place during preparation were characterised using real-time FTIR, dynamic light scattering and gel permeation chromatography. The solution characteristics were evaluated, using viscosimetry, followed by measurements of the thermal stability determined by thermogravimetric analysis. The optimal temperature for the condensation reaction was determined with the help of high-pressure differential scanning calorimetry. Once deposited on aluminium alloy 7075-T6 substrates, the coatings were evaluated using a field-emission scanning electron microscope coupled to an energy-dispersive spectrometer to determine surface morphology, topography, composition and coating thickness. Corrosion properties were tested in dilute Harrison's solution (3.5 g/L $(NH_4)_2SO_4$ and 0.5 g/L NaCl) using electrochemical impedance spectroscopy. The copolymerisation of MMA and MAPTMS over 4 h was optimal for obtaining 1.4-µm-thick coating with superior barrier protection against corrosion attack ($|Z_{10mHz}|$ ~ 1 GΩ cm^2) during three months of exposure to the corrosive medium.

Acrylate-based polysiloxane hybrid sol-gel coatings were synthesized using two different precursors, i.e., methyl- or ethyl- methacrylate (MMA or EMA), as corrosion protection of aluminium alloy 7075-T6. The hypothesis was that the additional alkyl group might affect the chemical properties and, consequently, the corrosion properties. The

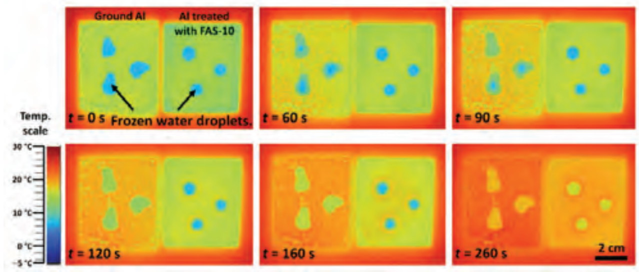

Figure 8: Frames of de-icing process on ground and treated surface after various times after taking the samples from the freezer (–15 °C) to ambient temperature followed using thermal infrared camera.

synthesis of the sols proceeded in two steps, each involving either MMA or EMA in the same molar ratio. The resulting sols, siloxane-(poly(methyl methacrylate-*co*-MAPTMS)) or siloxane-(poly(ethyl methacrylate-*co*-MAPTMS)), were applied on the aluminium alloy followed by characterization in terms of chemical structure and composition, topography, wettability, adhesion and corrosion resistance in 0.1 M sodium chloride solution. Coatings were similar in terms of surface topography, while the wettability of the coating with EMA showed a 6° greater water contact angle compared to the coating with MMA. Both coatings were shown, by electrochemical impedance spectroscopy in 0.1 M NaCl solution, to act as barriers to protect the underlying substrate in which coating with EMA exhibits better protection properties after 2 months of immersion. Adhesion tests confirmed the highest grade of adhesion to the substrate for both coatings. Testing in a salt-spray chamber demonstrated excellent corrosion protection, where coatings remaining intact after more than 600 h of exposure.

Sol-gel methodology offers many possibilities for the synthesis of coatings with various functional properties. One of them is hydrophobicity, which is then the basis for applications such as self-cleaning and anti-icing. A combination of the chemical etching process in $FeCl_3$ solution and chemical surface grafting by immersion in ethanol solution containing the 1H, 1H, 2H, 2H-perfluorodecyltriethoxysilane is a viable route to achieve a hierarchical surface topography and chemical bonding of silane molecules on aluminium surface leading to (super)hydrophobic characteristics. Characterisation of the untreated and treated aluminium surface was carried out using a contact profilometry, an optical tensiometry, scanning electron microscopy coupled with energy-dispersive spectroscopy and X-ray photoelectron spectroscopy to define the surface topography, wettability, morphology and surface composition. Additionally, the dynamic characteristics were evaluated to define the bouncing and the self-cleaning effect. The thermal infrared camera was employed to evaluate anti-icing properties (Figure 8). Nano-/micro-structured etched aluminium surface grafted with perfluoroalkyl silane film showed excellent super-hydrophobicity and bounce dynamics of a water droplet. A superhydrophobic aluminium surface exhibits the efficient self-cleaning ability of solid pollutants as well as improved anti-icing performance with melting delay.

Figure 9: (a) Objective of the KET4CP project was to consider the cleaning of metal surface by (b) a dry-ice process by the company FerroČrtalič instead of chemical cleaning. (c) Testing of steel samples covered by isocyanate-free coatings developed in collaboration with the company Chemcolor d.o.o.

In 2020 we intensively collaborated with industrial partners within the framework of Micro Grant KET4CP (Key Enabling Technology for Clean Production) of the Horizon 2020 programme. In the project entitled "Advanced environmentally friendly surface treatment for aluminium and aluminium alloys used in aircraft industry" together with company FerroČrtalič and Joanneum Research Institute from Austria we investigated the possibility to use alternative pre-treatments instead of chemical pre-treatment. The innovative technological solution introduced shot peening and dry-ice cleaning into pre-treatment technology to enhance the mechanical properties and corrosion protection obtained with ZrCC. These technologies are low-cost, easy-to-use and non-hazardous to the environment and reduce the reliance on raw materials as these novel processes (Figure 9). Used materials can be recycled and reused in the system. The developed technological solution can have a cross-border industry impact on other manufacturing companies, thus increasing their competitiveness and reducing the generation of pollution. Together with company Gabrijel Aluminium d. o. o. and Iberian Nanotechnology Laboratory (INL) from Portugal we worked on the project entitled "Surface-treatment process implementation for aluminium sealing to improve anti-corrosion properties". The objective was to investigate novel solutions for anodizing and sealing. Anodisation is one of the most commonly used surface pre-treatments of various aluminium and aluminium alloys. Due to several environmental restrictions on the use of chromate coatings, such a process is becoming the technology of choice for a number of markets. The pre-treatment formulation is affected by stricter environmental EU regulations (e.g., REACH) and standards of durability tests (ISO 9227). Moreover, the continued development of a more environmentally acceptable and more efficient anodisation process will drive the surface pre-treatment for enhanced corrosion protection in the automotive industry.

In the project entitled "Novel technological solution for the manufacturing of isocyanate-free polyurethane-based coatings used for corrosion protection of various metals" together with the company Chemcolor d.o.o. and Bay Zoltán Nonprofit Ltd. From Hungary we developed new alternatives based on organically modified silane precursors. The polyurethane technology market is very important for coating manufacturers. The coating formulation is affected by tighter volatile organic chemical (VOC) regulations and iso-cyanate. Moreover, the continued development of higher solids, low viscosity resins and curing agents coupled with higher performance characteristics, will drive the polyurethanes industry. The current coating systems often contain environmentally and human hazardous chemicals/components. One of them are isocyanates which are added into many coating systems to achieve final polymerisation between the functional groups in the coatings processes (Figure 9). Nowadays, the challenge is the preparation of ''green'', non-porous, isocyanate-free coatings. The replacement of isocyanates with a suitable alternative will make the production process cleaner and will reduce the pollution of the environment. The impact of the significantly improved technology was twofold: (i) environmental due to the use of environmentally friendly curing agents and (ii) economic due to possibility to increase sales of "greener" final product.

Organic synthesis of new compounds

We discovered that N-halosuccinimides in sub-stoichiometric amounts (1–7 mol.%) could be used as activators for several alcohols to promote the nucleophilic displacement of hydroxyl functional group and in the presence of various nucleophilic species enable the formation of new C–C, C–O, C–N or C–halogen bonds in target molecules. The best results were obtained using N-iodosuccinimide as the promotor and benzylic alcohols as the targets, while reactions could be performed under solvent-free reaction conditions.

The discovery was intensively evaluated in the case of direct cross-coupling of alcohols and C-nucleophiles, enabling the introduction of a new C–C bond in the target alcohols. The best results were obtained by electron-rich alkenes, such as 1,1-diphenylethenes, or 1,3-dicarbonyl compounds, which possess the electron-rich position C-2.

Some outstanding publications in the past year

1. I. Milošev, D. Zimerl, Ch. Carrièrre, S. Zanna, A. Seyeux, J. Iskra, S. Stavber, F. Chiter, M. Poberžnik, D. Costa, A. Kokalj, P. Marcus, The effect of anchor group and alkyl backbone chain on performance of organic compounds as corrosion inhibitors for aluminum investigated using an integrative experimental-modeling approach, Editor's Choice, J. Electrochem. Soc. 167 (2020) 061509.
2. G. Šekularac, I. Milošev, Electrochemical behavior and self-sealing ability of zirconium conversion coating applied on alumnum alloy 3005 in 0.5 M NaCl solution, J. Electrochem. Soc. 167 (2020) 021509.
3. M. Poberžnik, F. Chiter, I. Milošev, P. Marcus, D. Costa, A. Kokalj, DFT study of *n*-alkyl carboxylic acids on oxidized aluminium surfaces: From standalone molecules to self-assembled-monolayers, Appl. Surf. Sci., 525 (2020) 146156
4. P. Rodič, M. Lekka, F. Andreatta, L. Fedrizzi, I. Milošev, The effect of co-polymerization on the performance of acrylate-based hybrid so-gel coating for corrosion protection of AA2024-T3, Prog. Org. Coat., 147 (2020) 105701.
5. P. Rodič, B. Kapun, M. Panjan, I. Milošev, Easy and fast fabrication of self-cleaning and anti-icing perfluoroalkyl silane film on aluminium, Coatings, 10 (2020) 234.
6. M. Poberžnik, A. Kokalj, Surprising lateral interactions between negatively charged adatoms on metal surfaces, J. Phys. Chem. Lett., 11 (2020) 7122.

Awards and Appointments

1. Matjaž Dlouhy, First prize in the category best posters and lectures for the poster entitled "Adsorption of imidazole on Cu (111), covered with corrosion-important species" at the 26th annual meeting of the Slovenian Chemical Society entitled "Slovenian Chemical Days 2020", September 16–18, 2020.
2. Dr. Klara Čebular, Krka Award 2020 for her PhD thesis entitled 'Transformations of oxygen functional groups in organic molecules mediated by molecular iodine or/and N-halo compounds".

INTERNATIONAL PROJECTS

1. Advanced environmentally friendly surface treatment for aluminium and aluminium alloys used in the aircraft industry
Prof. Ingrid Milošev
Ferročrtalič d. o. o.
2. Surface treatment process implementation for aluminium sealing to improve anti-corrosion properties
Dr. Peter Rodič
Gabrijel Aluminium d. o. o.
3. Novel technological solution for the manufacturing of isocynate-free polyurethane-based coatings used for corrosion protection of various metals
Dr. Peter Rodič
Chemcolor d.o.o.
4. COST CA17126: Towards Understanding and Modelling Intense Electronic Excitation
Prof. Anton Kokalj
Cost Association Aisbl
5. 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
6. H2020 - MAMI; Magnetics and Microhydrodynamics - From Guided Transport to Delivery
Prof. Ingrid Milošev
European Commission

RESEARCH PROGRAMMES

1. Chemistry for sustainable development
Dr. Peter Rodič
2. Advanced materials for low-carbon and sustainable society
Prof. Ingrid Milošev

R & D GRANTS AND CONTRACTS

1. Modulation of polyketid synthase complex involved in early and late stages of tetracycline biosynthesis
Dr. Peter Rodič
2. Multidisciplinary approach towards development of a novel multifunctional

heterogeneous catalyst for efficient conversion of H2 and CO2 gas mixtures into fuel additives and surrogates
Prof. Anton Kokalj
3. Photocatalytic water treatment - development of immobilized catalysts and compact reactor systems
Dr. Peter Rodič
4. „COIN DESC: Corrosion inhibition and dealloying descriptors"
Prof. Anton Kokalj
Ministry of Education, Science and Sport

VISITORS FROM ABROAD

1. Dr. Emilie Gaudry, Institut Jean Lamour, University of Lorraine, Nancy, France, 3. 2. – 5. 2. 2020
2. Dr. Thiago Trevizam Dorini, Institut Jean Lamour, University of Lorraine, Nancy, France, 3. 2. – 14. 2. 2020

STAFF

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2. **Prof. Ingrid Milošev, Head**
3. Dr. Peter Rodič

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4. Dr. Matic Poberžnik
5. Dr. Gavrilo Šekularac
6. *Dr. Urša Tiringer, left 02.12.20*

Postgraduates
7. Matjaž Dlouhy, B. Sc.
8. *Damir Hamulić, B. Sc., left 01.07.20*
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13. Barbara Kapun, B. Sc.
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Original Article

1. Marjan Bele *et al.* (12 authors), "Increasing the oxygen-evolution reaction performance of nanotubular titanium oxynitride-supported Ir nanoparticles by a strong metal–support interaction", *ACS Catalysis*, 2020, **10**, 22, 13688-13700.
2. Vesna Ribić, Aleksander Rečnik, Matej Komelj, Anton Kokalj, Zorica Branković, Mario V. Zlatović, Goran Branković, "New inversion boundary structure in Sb-doped ZnO predicted by DFT calculations and confirmed by experimental HRTEM", *Acta Materialia*, 2020, **199**, 633-648.
3. Anton Kokalj, Hadi Behzadi, Razieh Farahati, "DFT study of aqueous-phase adsorption of cysteine and penicillamine on Fe(110): role of bond-breaking upon adsorption", *Applied Surface Science*, 2020, **514**, 145896.
4. Matic Poberžnik, Fatah Chiter, Ingrid Milošev, Philippe Marcus, Dominique Costa, Anton Kokalj, "DFT study of *n*-alkyl carboxylic acids on oxidized aluminum surfaces: from standalone molecules to self-assembled-monolayers", *Applied Surface Science*, 2020, **525**, 146156.
5. Damir Hamulić, Peter Rodič, Matic Poberžnik, Marjan Jereb, Janez Kovač, Ingrid Milošev, "The effect of the methyl and ethyl group of the acrylate precursor in hybrid silane coatings used for corrosion protection of aluminium alloy 7075-T6", *Coatings*, 2020, **10**, 2, 172.
6. Peter Rodič, Barbara Kapun, Matjaž Panjan, Ingrid Milošev, "Easy and fast fabrication of self-cleaning and anti-icing perfluoroalkyl silane film on aluminium", *Coatings*, 2020, **10**, 3, 234.
7. Gavrilo Šekularac, Janez Kovač, Ingrid Milošev, "Prolonged protection, by zirconium conversion coatings, of AlSi7Mg0.3 aluminium alloy in chloride solution", *Corrosion Science*, 2020, **169**, 108615.
8. Barbara Volarič, Anca Mazare, Sannakaisa Virtanen, Ingrid Milošev, "The effect of deposition parameters on the properties of $CeCl_3$ and $LaCl_3$ conversion coatings deposited on three Al-based substrates", *Corrosion*, 2020, **76**, 1, 18-38.
9. Matic Poberžnik, Anton Kokalj, "Surprising lateral interactions between negatively charged adatoms on metal surfaces", *The Journal of Physical Chemistry Letters*, 2020, **11**, 17, 7122-72126.
10. Gavrilo Šekularac, Ingrid Milošev, "Electrochemical behavior and self-sealing ability of zirconium conversion coating applied on aluminum alloy 3005 in 0.5 M NaCl solution", *Journal of The Electrochemical Society*, 2020, **167**, 2, 021509.
11. Ingrid Milošev *et al.* (12 authors), Editors' choice –"The effect of anchor group and alkyl backbone chain on performance of organic compounds as corrosion inhibitors for aluminum investigated using an integrative experimental-modeling approach", *Journal of The Electrochemical Society*, 2020, **167**, 6, 061509.
12. Gavrilo Šekularac, Janez Kovač, Ingrid Milošev, "Comparison of the electrochemical behaviour and self-sealing of zirconium conversion coatings applied on aluminium alloys of series 1xxx to 7xxx", *Journal of The Electrochemical Society*, 2020, **167**, 11, 111506.
13. Peyman Taheri, Ingrid Milošev, Mats Meeusen, Barbara Kapun, Paul White, Anton Kokalj, Arjan Mol, "On the importance of time-resolved electrochemical evaluation in corrosion inhibitor-screening studies", *npj Materials Degradation*, 2020, **4**, 12.
14. Peter Rodič, Romana Cerc Korošec, Barbara Kapun, Alenka Mertelj, Ingrid Milošev, "Acrylate-based hybrid sol-gel coating for corrosion protection of AA7075-T6 in aircraft applications: the effect of copolymerization time", *Polymers*, 2020, **12**, 4, 948.
15. Peter Rodič, Maria Lekka, Francesco Andreatta, Lorenzo Fedrizzi, Ingrid Milošev, "The effect of copolymerisation on the performance of acrylate-based hybrid sol-gel coating for corrosion protection of AA2024-T3", *Progress in Organic Coatings*, 2020, **147**, 105701.
16. Peter Rodič, Ingrid Milošev, "Corrosion resistance of cerium-conversion coatings formed from cerium(III) salts on aluminium alloy 7075-T6", *Studia Universitatis Babeş-Bolyai. Chemia*, 2020, **65**, 3, 227-244.

Published Conference Contribution

1. Dirk Lützenkirchen-Hecht, Damir Hamulić, Ralph Wagner, Ingrid Milošev, "EXAFS investigations of cobalt electrodeposition", In: *XAFS2018, 17th International Conference on X-ray Absorption Fine Structure, 22-27.07, 2018, Kraków, Poland*, Proceedings, (Radiation physics and chemistry **175**), 2020, 108113.

Theses and Mentoring

1. Gavrilo Šekularac, *Corrosion and corrosion protection of aluminium alloys by zirconium conversion coatings:* doctoral dissertation, Ljubljana, 2020 (mentor Ingrid Milošev).

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 and conductive oxides. The emphasis is on the creation of the properties through synthesis and structure on the nano-, micro- and macro-levels. The group also works on the principles of basic technologies of ceramic pressure sensors, ceramic MEMS and flexible electronics.

Head:

Prof. Barbara Malič

In the framework of **lead-free piezoelectric ceramics**, we continued the research of sodium potassium niobate **($K_{0.5}Na_{0.5}NbO_3$, KNN) based** materials, which could replace efficient lead-based piezoelectrics. The focus has been on the control of chemical homogeneity in multi-metal-modified KNN ceramics as the key to achieving reproducible functional properties.

We continued with the work on **polycrystalline $BiFeO_3$**. In collaboration with researchers from the Department for Nanostructured Materials (Jožef Stefan Institute, JSI), and the National Institute of Chemistry, using a combined characterisation of $BiFeO_3$ on the nano and atomic scales, we revealed a pinning mechanism associated with conductive domain walls (DWs), whose origin lies in the dynamic coupling of the p-type defects gathered in the DW regions with the DW displacements under an applied electric field. We confirmed that the degree of defect ordering at the walls, which affect the DW local structure and conductivity, can be tuned by the cooling rate used during the annealing [Figure 1].

The study that reveals a unique dynamic response of relaxor ferroelectrics to external fields, reflecting their complex structure in terms of the hierarchical texture of ferroelectric domains on top of the disorder at the atomic scale, both of which strongly affect the mobility of the domain walls, was published in the journal *Advanced Functional Materials.*

Owing to the high electrical conductivity and coercive field, the poling of $BiFeO_3$ ceramics is notoriously difficult. In collaboration with colleagues from Australia (University of New South Wales), China (Tsinghua University) and Norway (Norwegian University of Science and Technology), we performed in-situ structural X-ray diffraction analysis that aimed to understand the poling behaviour of $BiFeO_3$. A peculiar inverse time-dependent trend in the microstrain and non-180° domain texture was observed during poling, attributed to the effect of conductive domain walls in redistributing the internal electric fields inside the grains of the ceramics. The results clarify, for the first time, the microstrain mechanisms in $BiFeO_3$ during static field loading and act as a guideline for tailoring local conductivities in view of the poling behaviour and the post-poling strain relaxation.

Experimental studies on $BiFeO_3$ ceramics modified with a controlled amount of cobalt ions revealed details of the ferroelectric hardening behaviour of this perovskite. The data show two distinct hardening mechanisms related to i) domain-wall pinning effects arising from oxygen-vacancy defect complexes, which are known to dominate the hardening behaviour of hard $Pb(Zr,Ti)O_3$ (PZT), and ii) less-common pinning effects associated with the accumulation of electronic defects inside DW regions. The mechanism (i) plays a dominant role in the polarization switching properties of $BiFeO_3$ at high electric fields, while the mechanism (ii) has a crucial effect on the weak-field piezoelectric response of $BiFeO_3$. In particular, the charges present at domain walls lead to a counterintuitive enhancement of the piezoelectric response of $BiFeO_3$. This happens due to a re-distribution of the internal fields in different grain-families of the polycrystalline matrix, triggered by the charge migration along the domain walls, which effectively enhances the domain-wall contribution in those grains in which the field is increased. The results explain the long-standing question of the complex hardening behaviour of $BiFeO_3$ and provide the means for its control with cobalt or similar acceptor dopants.

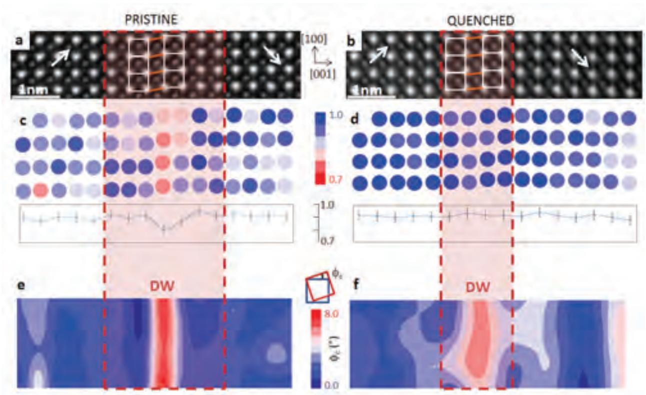

*Figure 1: Atomic structure of domain walls (DWs) in pristine and quenched $BiFeO_3$.
HAADF-STEM image of a 109° DW in (a) pristine and (b) quenched $BiFeO_3$ with corresponding (c, d) normalized distribution map of Bi-column intensities and average intensity profiles across the DW region and (e,f) lattice-strain maps represented in terms of lattice-distortion angle (φc). The DW region is indicated by a dashed red box. In panels (a,b) the arrows indicate the direction of the Fe displacements from the centre of the Bi sublattice; enlarged distances between the sheared Bi atoms columns (shear lattice strain) inside the DWs are indicated by red lines.*

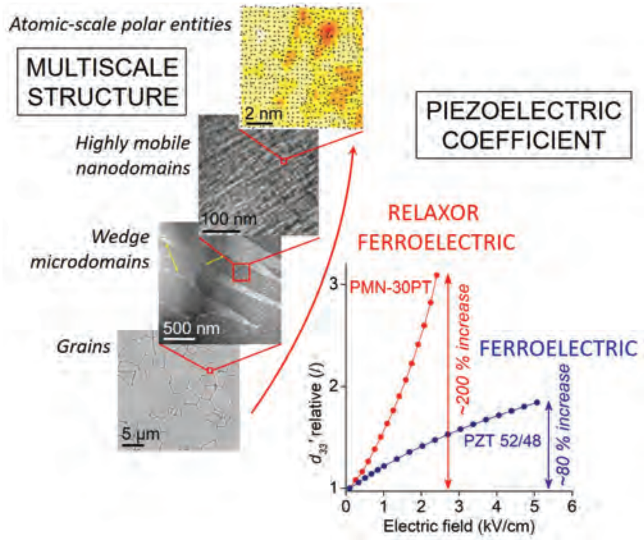

Figure 2: Anomalously large nonlinear piezoelectric response is identified in relaxor ferroelectric PMN-xPT ceramics, revealing a previously unrecognized softening mechanism arising from the highly mobile nanodomain walls, facilitated by the nanoscale polar character and lattice strain disorder, common to relaxors.

A study that reports on a pinning mechanism associated with conductive DWs, whose origin lies in the dynamic coupling of the p-type defects gathered in the DW regions with the DW displacements under an applied electric field, was published in the journal *Nature Communications.*

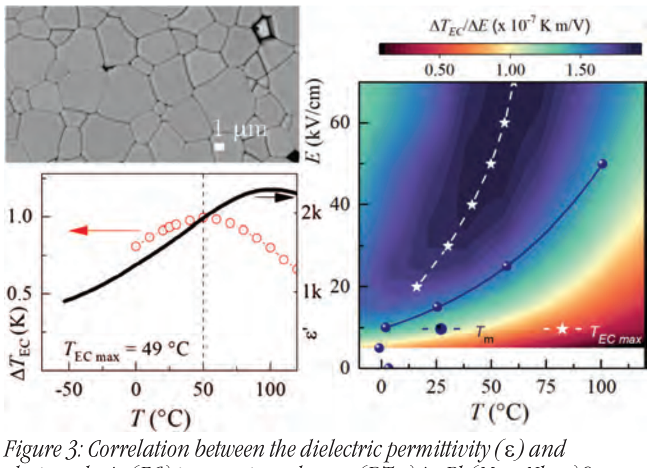

Figure 3: Correlation between the dielectric permittivity (ε) and electrocaloric (EC) temperature change (DT_{EC}) in $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN). Left: microstructure of PMN (top) and temperature dependence of ε (@10 kHz) and DT_{EC} at the applied field of 50 kV/cm revealing that the peak of the dielectric permittivity (T_m) is at a higher temperature than the maximum DT_{EC}. Right: EC responsivity ($DT_{EC}/\Delta E$) in the frame of the electric field–temperature phase diagram of PMN.

In collaboration with colleagues from the Norwegian University of Science and Technology, Trondheim, Norway and from the National Institute of Research and Development for Technical Physics, Iasi, Romania, we investigated the magnetic properties of multiferroic $Bi_{0.88}Gd_{0.12}FeO_3$ ceramics. Using piezo-response force microscopy (PFM) and magnetic force microscopy (MFM) we confirmed the intrinsic multiferroicity in the perovskite phase with the coexistence of ferroelectric/ferroelastic and ferromagnetic domains. A strong magnetic hysteresis and high magnetization were produced by heating the sample to 1000 °C due to degeneration of the perovskite phase into iron oxide inclusions. These results highlighted the importance of sample processing, thermal history and the thermodynamic stability of secondary phases when considering the magnetic performance of $Bi_{0.88}Gd_{0.12}FeO_3$ ceramics.

In collaboration with colleagues from the Technical University of Darmstadt in Germany we prepared and characterized **lead-based piezoelectric ceramics** $Pb(Zr_{0.7}Ti_{0.3})O_3$ with grain sizes in the range 3.9 to 10.4 μm. A decrease in the grain size was accompanied by a reduction in the electromechanical properties at switching fields and an increase in the relative permittivity. The PFM analysis indicated an increased local coercive voltage near the grain boundaries. The grain-size-dependent changes in the properties were related to the strained material volume close to the grain boundaries exhibiting reduced DW dynamics.

Despite numerous proposed models and diverse explanations, the origins of the high piezoelectricity in **lead-based relaxor ferroelectrics**, exemplified by $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT), are still under debate. Using a multiscale analytical approach and a wide range of PMN-PT ceramic compositions, we managed to explain a piece of the puzzle, showing the key role of the so-called, low-angle domain walls to the extrinsic piezoelectric and dielectric response of PMN-PT. The high mobility of these interfaces is intimately linked to the relaxor disorder, hence their dynamics dominate the response of monoclinic PMN-rich compositions. The study was performed in collaboration with colleges from the Department of Systems and Control (JSI), the National Institute of Chemistry, the North Carolina State University, USA, and the Swiss Federal Institute of Technology in Lausanne, Switzerland. The new softening mechanism opens up a plethora of possibilities for designing high-performance piezoceramics via relaxor disorder [Figure 2].

In collaboration with colleagues from the Condensed Matter Department, JSI, and the Technical University of Darmstadt, Germany, we studied the correlation between the dielectric permittivity and the electrocaloric (EC) temperature change (DT_{EC}) in (1-x)$Pb(Mg_{1/3}Nb_{2/3})O_3$–x$PbTiO_3$ (PMN-100xPT, with x = 0, 0.05, and 0.10). Both the peak permittivity temperature and the temperature at which the DT_{EC} is the highest, increased with increasing PT content for a given electric field (E). The peak of the dielectric permittivity is always at a higher temperature than the maximum DT_{EC} and the temperature gap between both maxima progressively increases with an increasing applied field. This is even more evident above the threshold field, which induces the long-range-ordered ferroelectric state. The results are explained in the frame of the electric field–temperature phase diagram of relaxor systems. Our study revealed that the temperature of the peak permittivity only roughly indicates the temperature of the upper boundary of the temperature–electric field window where the EC responsivity ($DT_{EC}/\Delta E$) is the highest [Figure 3].

We proceeded with the preparation and investigation of new **$Pb(Fe_{0.5}Nb_{0.5})O_3$-based** single-phase **multiferroic and multicaloric ceramic** materials. The $Pb(Fe_{0.5}Nb_{0.5})O_3$–$BiFeO_3$ (PFN–BFO) solid solutions offer a bridge between the low-temperature phase transitions of PFN and the high-temperature phase transitions of BFO, which enables the tailoring of the multiferroic properties. Several

(1-x)PFN–xBFO (x = 0–0.5) compositions were prepared by mechanochemical synthesis from constituent oxides, followed by thermal treatment. The addition of BFO to PFN led to an enhanced relaxor-like behavior, which was systematically investigated using a wide range of macroscopic and local characterization techniques [Figure 4]. In addition to promising relaxor-ferroelectric properties, the PFN–BFO system also exhibits magnetic properties. The 0.8PFN–0.2BFO composition possesses both ferroic anomalies at room temperature, and is therefore one of the first single-phase multiferroic materials. Further investigation of caloric properties revealed its multicaloric nature, and with the targeted doping of 0.8PFN–0.2BFO with Gd and Mn ions resulting in the coexistence of the highest electrocaloric and magnetocaloric effects to date in a single-phase material.

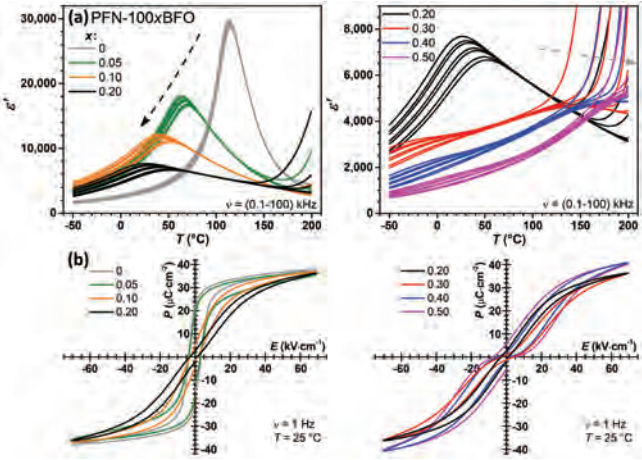

Figure 4: Pb(Fe$_{0.5}$Nb$_{0.5}$)O$_3$–BiFeO$_3$ (PFN–BFO) solid solutions (a) Temperature and frequency dependences of the real component of relative permittivity, (b) P–E hysteresis loops.

In collaboration with researchers from Canada (McMaster University and Université de Sherbrooke) and the USA (Oak Ridge National Laboratory) we carried out a comprehensive study of underdoped and overdoped $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ **cuprate superconductors**. We were able to map the structural and superconducting phase transitions that take place as a function of temperature and hole doping, p, and to propose an updated temperature–doping phase diagram for $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$. In addition, we also found out that the structural and pseudogap critical points are well separated in this system, similar to the parent compound, $La_{1-x}Sr_xCuO_4$.

Another focus of our research was on the double perovskite La_2LiMoO_6. Our study performed in collaboration with scientists from the Oak Ridge National Laboratory, University of Tennessee, USA, and McMaster University and University of Winnipeg, Canada, elucidated the magnetic ground state in this material. In contrast to other Mo^{5+} double perovskites, we found that La_2LiMoO_6 is the first one showing long-range **antiferromagnetic** order with a T_N of 18 K, as evidenced by resolution-limited magnetic Bragg peaks. These differences might be explained on the basis of the Mo-O coordination polyhedra that further determines the nature of the orbital ordering.

Hybrid **organic-inorganic ferroelectrics**, such as those based on tetramethylammonium bromotrichloroferrate ($N(CH_3)_4[FeBrCl_3]$), hold promises as the next generation of functional materials for sensing and energy-harvesting applications. While these so-called plastic crystals are structurally well understood, their essential ferroelectric and electromechanical properties are largely unknown. Through a collaboration with the group from the Norwegian University of Science and Technology in Trondheim we characterized and recently reported the functional properties of N(CH3)4[FeBrCl3] plastic crystals. The data suggested a classic ferroelectric response arising from domain switching with a contribution from leakage current observed in the low-frequency polarization response. The strong dependence of the strain response on the driving frequency and field cycling indicated pinning effects mediated by point defects. The results highlight the need for a further investigation of the defect chemistry in this promising group of hybrid materials.

The achievement Innovative approaches to controlled functional responses of multiferroics was selected for 'Excellent in Science 2020' recognition by Slovenian Research Agency. It is the result of collaboration of researchers from Departments of Electronic Ceramics, Condensed Matter Physics, Nanostructured Materials (JSI), National Institute of Chemistry, and colleagues from Poland and the US.

In collaboration with the Department for Gaseous Electronics (JSI) we investigated the ferroelectric domain structure of undoped and Cu-doped $Sn_2P_2S_6$ single crystals by PFM. In both cases a-few-hundred-nanometres-large ferroelectric domains were observed; however, in the undoped samples, the domains were more rhombus-like with sharp edges, while in Cu-doped samples the domains were more irregular in shape. The PFM amplitude and phase hysteresis loops indicated a good domain-switching ability of both types of single crystals.

In collaboration with the Institute for Multidisciplinary Research, University of Belgrade, Serbia, we studied the influence of strontium doping on the phase composition, microstructure and functional properties of **sodium potassium niobate thin films**. The solution-derived films were deposited on platinized silicon substrates and rapid thermally annealed. Sr-doping (0.5, 1 mol%) contributed to the fine-grained and dense thin-film microstructure, and improved ferroelectric characteristics. Benefiting from improved leakage current characteristics at high electric fields, the films showed a high local piezoelectric activity (d_{33} ~110 pm/V) determined by piezo-response force microscopy (PFM) and an ability to reach a fully saturated local hysteresis.

The research of piezoelectric thick films was performed in collaboration with researchers from the GREMAN/CNRS/University of Tours, France. We continued the study of the **electrophoretic deposition (EPD) of thick films** for the processing of environmentally benign $(K_{0.5}Na_{0.5})_{0.99}Sr_{0.005}NbO_3$ (KNNSr) thick films on metalized ceramic substrates for energy harvesting. The dielectric, ferro- and piezoelectric properties of the thick films increased with the increasing sintering temperature, regardless of the sintering atmosphere. The KNNSr thick films sintered at 1100 °C for 2 hours in oxygen were 28 µm thick with k_t of 40 %, similar to that for a bulk ceramic with the same nominal composition.

We continued with the processing of $Pb(Zr,Ti)O_3$ (PZT) based thick-film structures by **piezoelectric inkjet printing**, a computer-controlled, low-cost and environmentally benign patterning technology. By adjusting the surface tension, viscosity and wetting properties of the aqueous suspension (ink) and the printing conditions, we prepared uniform, defect-free patterns with dimensions of 4 mm × 4 mm on metalized alumina substrates. After sintering at 850 °C the 15-µm-thick film with a relative density of 86 % and a grain size up to ~2 µm had an effective thickness coupling factor k_t of 46 %, which is comparable to that of the bulk ceramic.

Prof. Barbara Malič received the Zois Award for achievements in the research of electrocaloric ceramic materials.

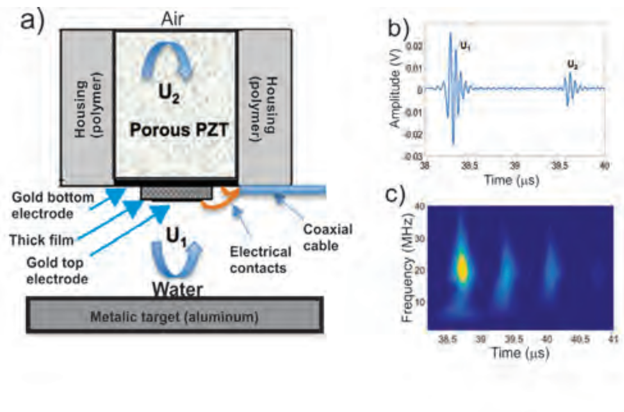

Figure 5: a) Schematic of the acoustic measurements of ultrasound transducer at frequencies over 10 MHz; b) time responses (U1 and U2 signals) and c) its wavelet transforms (c).

Together with colleagues from Tours, we developed a prototype of a miniature, high-frequency ultrasonic transducer and established a method for measuring the acoustic properties of backing in water in the frequency range of 15 to 25 MHz. We were the first to report on this effective method. The transducer consisted of a PZT thick film and a gold electrode that were screen-printed on a backing. The backing consisted of a porous PZT ceramic, and was fabricated by a sacrificial template method combined with a hetero-coagulation process. The backing with 30 % porosity and spherical pores with a diameter of 10 µm had an attenuation coefficient α of 33 dB/mm at 19 MHz, which is three times higher than the values reported in the literature. The PZT backing with a high value of α effectively dampens the ultrasonic waves, which makes it possible to reduce its thickness and thus the total size of the transducer suitable for medical investigations [Figure 5].

We continued with the preparation of **thick films using the aerosol deposition method**. The aerosol deposition system is a part of the Laboratory for the ultracool preparation of complex oxides, for which financial support was granted by **the Director's fund ULTRACOOL project**. In April 2020 the project was successfully completed [Figure 6]. Current research related to aerosol deposition is focused on the optimization of processing parameters of functional PMN-PT thick films on metal and polymer substrates.

In the scope of the ULTRACOOL laboratory, the dedicated cold-sintering press made it possible to perform a series of sintering experiments of the effects of pressure, temperature and liquids used in a **cold-sintering** process of the multiferroic BFO ceramic. The optimization of parameters led to ceramics with improved properties compared to the conventional high-temperature sintering from the inclusion of a secondary phase point of view, as well as lower conductivity and larger field-induced strains.

The aerosol deposition method was the main method used in the frame of a **European project** Key Enabling Technologies for Clean Production **KET4CP** - *Alternative process for producing metal electrodes on ceramic electronic components* with the partners Stelem d.o.o., Slovenia, Bay Zoltán Nonprofit Ltd., Hungary, and the JSI.

In the **KET4CP** project "Developing a new clean manufacturing process for ceramic pressure sensors" the partners KEKO Equipment, Slovenia, Hahn-Schickard, Germany and JSI a ceramic pressure-sensing element with the operation up to 500 °C was designed, developed and successfully tested. Compared to the conventional alumina-based sensing elements the use of LTCC (Low-Temperature Co-fired Ceramic) materials and technology leads to a 'cleaner' manufacturing process based on lower energy and material consumption, and reduced generation of waste and pollution.

In 2020, two European KET4CP projects, in which we were developing new products and technologies for Slovenian companies, were successfully concluded.

In the **KET4CP** project "Manufacturing of invisible interconnections from solutions of low-cost transparent conduction oxides by screen printing" we collaborate with RC eNeM, Slovenia and Institute of Solid State Physics from Latvia. We have been studying procedures for the deposition of zinc-oxide-based films on glass from solution by Chemical Solution Deposition and screen-printing technology.

Some outstanding publications in the past year

1. Otoničar, Mojca, Bradeško, Andraž, Fulanović, Lovro, Kos, Tomaž, Uršič Nemevšek, Hana, Benčan, Andreja, Cabral, Matthew, Henriques, Alexandra, Jones, Jacob L., Riemer, Lukas, Damjanović, Dragan, Dražić, Goran, Malič, Barbara, Rojac, Tadej. Connecting the multiscale structure with macroscopic response of relaxor

ferroelectrics. **Advanced functional materials**, ISSN 1616-301X, [in press] 2020, 13 str., doi: 10.1002/adfm.202006823. [COBISS.SI-ID 32051715]

2. Benčan, Andreja, Dražić, Goran, Uršič Nemevšek, Hana, Makarovič, Maja, Komelj, Matej, Rojac, Tadej. Domain-wall pinning and defect ordering in $BiFeO_3$ probed on the atomic and nanoscale. **Nature communications**, ISSN 2041-1723, 2020, vol. 11, str. 1762-1-1762-8, doi: 10.1038/s41467-020-15595-0. [COBISS.SI-ID 33296423]
3. Prah, Uroš, Dragomir, Mirela, Rojac, Tadej, Benčan, Andreja, Broughton, Rachel, Chung, Ching-Chang, Jones, Jacob L., Sherbondy, Rachel, Brennecka, Geof, Uršič Nemevšek, Hana. Strengthened relaxor behavior in $(1-x)Pb(Fe_{0.5}Nb_{0.5})O_3xBiFeO_3$. **Journal of materials chemistry. C**, Materials for optical and electronic devices, ISSN 2050-7526. [Print ed.], 2020, vol. 8, no. 10, str. 3452–3462, doi: 10.1039/C9TC05883D. [COBISS.SI-ID 33157415]
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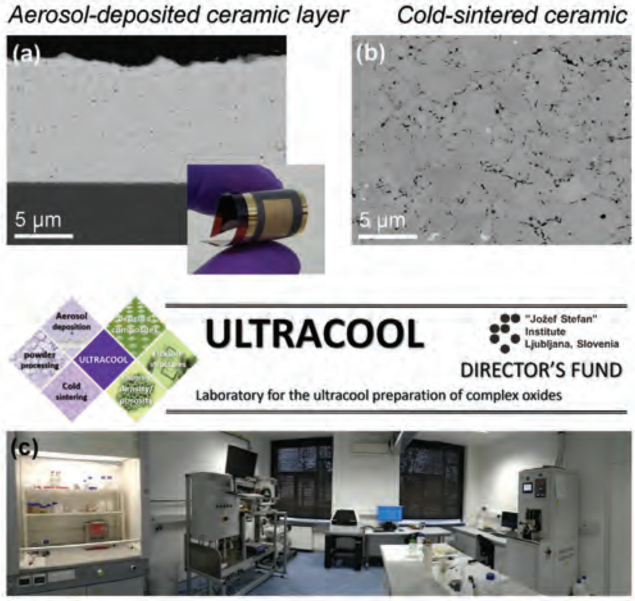

Figure 6: Successfully equipped and tested ULTRACOOL laboratory, supported by the 2017 Director's fund, for the preparation of functional materials at low temperatures. (a) dense ceramic layer prepared by aerosol deposition method. (b) Multiferroic $BiFeO_3$ ceramic prepared by the cold sintering method. (c) panoramic view of the laboratory.

Awards and Appointments

1. Andreja Benčan Golob, Andraž Bradeško, Mirela Dragomir, Goran Dražić, Maja Makarovič, Barbara Malič, Uroš Prah, Tadej Rojac, Hana Uršič Nemevšek: Achievement Excellent in Science 2020 for Innovative approaches to the control of functional responses of multiferroices, Slovenian Research Agency
2. Mirela Dragomir: Seal of Excellence for project application QMAT – Towards Quantum States of Matter via Chemistry under Ambient and Extreme Conditions, European Commission
3. Barbara Malič: Zois Award for top achievements in the field of electrocaloric ceramic, Government of the Republic of Slovenia

INTERNATIONAL PROJECTS

1. Minor Services - Foreign Customers
Prof. Barbara Malič
2. Laboratory Measurements
Prof. Barbara Malič
Tdk Electronics Gmbh & Co Og
3. Electrical Measurements
Prof. Tadej Rojac
Tdk Electronics Gmbh & Co Og
4. Laboratory Measurements
Prof. Andreja Benčan Golob
Tdk Electronics Gmbh & Co Og
5. Atomic Force Microscope Measurements
Asst. Prof. Hana Uršič Nemevšek
Tdk Electronics Gmbh & Co Og
6. Cold Sintering of Complex Oxide Materials
Dr. Mojca Otoničar
Slovenian Research Agency
7. Low Bandgap Ferroelectric Solar Cell Absorbers: Synthesis and Characterization
Asst. Prof. Hana Uršič Nemevšek
Slovenian Research Agency
8. Interface Stability of Piezoelectric Ceramic Oxides
Prof. Tadej Rojac
Slovenian Research Agency
9. Environmental Benign Sodium Potassium Niobate-based Thick Films for Piezoelectric Energy Harvesting Applications
Prof. Danjela Kuščer Hrovatin
Slovenian Research Agency
10. Understanding Size Effects in Antiferroelectric Materials
Dr. Mojca Otoničar
Slovenian Research Agency
11. Multiferroics for Solid-State Cooling Applications
Asst. Prof. Hana Uršič Nemevšek
Slovenian Research Agency
12. Processing – Structure - Properties Study of Environmentally Friendly Piezoelectric Nanoparticles of Tailored Surface Morphology
Prof. Andreja Benčan Golob
Slovenian Research Agency
13. High-Pressure Synthesis and Characterization of Selected Ferroics
Dr. Kristian Radan
Slovenian Research Agency
14. Crystal Growth and Magnetic Properties of Double Perovskites
Dr. Mirela Dragomir
Slovenian Research Agency
15. Porous Lead-Free Relaxor Ferroelectric Films for Energy Storage
Asst. Prof. Hana Uršič Nemevšek
Slovenian Research Agency
16. Environment-Friendly Ferroelectric Oxide Thin Films for Energy Harvesting and Energy Storage Applications
Prof. Barbara Malič
Slovenian Research Agency

17. 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
18. Engineering the Microstructure and Performance of Lead-Free Piezoelectrics for Energy Harvesting
Prof. Barbara Malič
Slovenian Research Agency
19. Environment-Friendly Processing of Lead-Free Functional-Oxide Thin Films for Micro-Electro-Mechanical Systems (MEMS) Applications
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. Multicaloric cooling
Asst. Prof. Hana Uršič Nemevšek
2. Electrocaloric elements for active cooling of electronic circuits
Prof. Barbara Malič
3. Advanced inorganic and organic thin films with enhanced electrically-induced response
Prof. Barbara Malič
4. The quest for high-temperature superconductvity and exotic magnetism in fluoridoargentates(II)
Dr. Mirela Dragomir
5. Designing functionality of lead-free ferroelectrics through domain wall engineering
Prof. Andreja Benčan Golob
6. The cool way to polarize
Dr. Mojca Otoničar
7. Engineering of relaxor ferroelectric thin films for piezoelectric and energy storage applications
Prof. Tadej Rojac
8. Domain engineered ferroelectric ceramic layer elements for efficient energy harvesting and energy conversion applications
Prof. Barbara Malič
9. Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF)
Prof. Barbara Malič
Ministry of Economic Development and Technology
10. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
Prof. Barbara Malič
Slovenian Research Agency
11. Stay of Oana Andreea Condurache in AI CUZA Iasi, Romania - Functional Characterisation of Potassium Sodium Niobate-Based and Bismuth Ferrite-Based Ceramics
Oana Andreea Condurache
Jecs Trust

NEW CONTRACTS

1. Developing clean manufacturing process for ceramic pressure sensors
Asst. Prof. Hana Uršič Nemevšek
Stelem d. o. o. Žužemberk
2. Developing clean manufacturing process for ceramic pressure sensors
Prof. Barbara Malič
Keko - Oprema d. o. o. Žužemberk
3. Development of new production process for manufacturing of invisible interconnections from solutions of low-cost transparent conduction oxides by screen printing
Prof. Danjela Kuščer Hrovatin
Razvojni center Enem Novi Materiali d. o. o.

VISITORS FROM ABROAD

1. Kristijan Kovačić, Bjelovar University of Applied Sciences, Bjelovar, Croatia, 16 September 2019 to 13 March 2020
2. Anja Mirjanić, University of Banja Luka, Faculty of Natural Sciences and Mathematics, Bosnia and Hercegovina, 17 October 2019 to 30 November 2020
3. Prof. Dragan Damjanovic, École polytechnique fédérale de Lausanne - EPFL, Lausanne, Switzerland, 5-11 January 2020
4. Dr Marco Deluca, Materials Center Leoben Forschung GmbH, Leoben, Austria, 9-11 January 2020
5. Vignaswaran Kaliyaperumal Veerapandiyan, Materials Center Leoben Forschung GmbH, Leoben, Austria, 9-11 January 2020
6. Konstantin Rokas, University of Ioannina, Ioannina, Greece, 13 January to 13 March 2020
7. Gianni Ferrero, Meggitt Sensing Systems, Kvistgaard, Denmark, 13 January 2020 to 16 March 2020 and 1–27 October 2020
8. Mustafa Çağrı Bayir, Gebze Technical University, Department of Materials Science and Engineering, Kocaeli, Turkey, 3 February to 12 March 2020
9. Katharina Schuldt, Techniche Universität Darmstadt, Darmstadt, Germany, 7–12 March 2020

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4. **Prof. Barbara Malič, Head**
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6. Prof. Tadej Rojac
7. Asst. Prof. Hana Uršič Nemevšek

Postdoctoral associates
8. *Dr. Andraž Bradeško, left 01.07.20*
9. Dr. Mirela Dragomir
10. Dr. Kostja Makarovič*
11. Dr. Kristian Radan

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14. Sabi William Konsago, B. Sc.
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22. Brigita Kmet, B. Sc.
23. *Marija Šebjan Pušenjak, B. Sc., left 01.10.20*

Technical and administrative staff
24. Tina Ručigaj Korošec, B. Sc.

Note:
* part-time JSI member

BIBLIOGRAPHY

Original Article

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1. Barbara Malič, Mojca Otoničar, Kristian Radan, Jurij Koruza, "Lead-free piezoelectric ceramics", In: *Reference module in materials science and materials engineering*, Elsevier, 2020.
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Theses and Mentoring

1. Vinko Grm, *Development of smart textile for heating application based on carbon nanotubes composite material:* doctoral dissertation, Ljubljana, 2020 (mentor Goran Dražić; co-mentor Daniela Zavec Pavlinić).
2. Maja Makarovič, *Defect chemistry and hardening of ferroelectric cobalt-doped bismuth ferrite ceramics:* doctoral dissertation, Ljubljana, 2020 (mentor Tadej Rojac; co-mentor Sverre Magnus Selbach).
3. Hugo Mercier, *Sodium potassium niobate-based thick films by electrophoretic deposition for piezoelectric energy harvesting:* doctoral dissertation, Ljubljana, 2020 (mentor Danjela Kuščer; co-mentor Franck Levassort).
4. Uroš Prah, *Combining electrocaloric and magnetocaloric effects in single-phase multiferroics:* doctoral dissertation, Ljubljana, 2020 (mentor Hana Uršič Nemevšek; co-mentor Tadej Rojac).

DEPARTMENT FOR NANOSTRUCTURED MATERIALS K-7

The research and development at the Department for Nanostructured Materials are focused on the forefront areas of nanotechnology and advanced materials to address 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 magnets and intermetallic alloys, engineering and functional ceramics, minerals, sensors, materials for a sustainable and ecologically built environment, biomimetic- and bio-materials.

Head:

Prof. Sašo Šturm

Magnetic Materials

For the transition to an energy-efficient and low-carbon society by 2050 set by "European Green Deal" we aim to reduce the greenhouse-gas emissions by 80%. The major contributing segments are the development of e-mobility and eco-power generation, requiring highly efficient electric motors that are based on rare-earth permanent magnets (Nd-Fe-B). However, the rare earths are subject to political and economic manipulation and are recognized by the EU as the most critical raw materials of strategic importance. Through research, we bring new knowledge to areas of design and the manufacture of new Nd-Fe-B magnets with improved magnetic properties either from raw materials or from recycled feedstocks. We also explore novel, economically feasible and environmentally friendly routes of recycling, thus contributing to EU sustainability.

We have developed a new process for recycling permanent Nd-Fe-B magnets, allowing the simultaneous selective extraction of the rare earths and the transition metals with a large reduction in energy consumption and environmental burden, as it operates in a closed loop, so it literally does not produce waste. The article will be published in the journal Green Chemistry and is the result of the recently completed ITN-MSCA-DEMETER project (Training Network for the Design Recycling of Rare-Earth Permanent-Magnet Motors and Generators in Hybrid and Full Electric Vehicles).

Editorial Board from the prominent journal Green Chemistry (IF= 9.346) has selected a paper by XU, Xuan, et al., "A facile method for the simultaneous recovery of the rare-earth elements and transition metals from Nd-Fe-B magnets" as a 2020 HOT Green Chemistry article. This new closed-loop technology of continuous process magnetic leaching and rare-earth recovery surpasses the current state-of-the-art method of hydrometallurgy in relation to the chemical usage, waste production and total costs and is under protection by a patent application at the European patent office, Application EP 19197716.4.

We correlated the magnetic properties of Tb-treated Nd-Fe-B PMs with a detailed microstructural study, via a paper on microstructural insights into the coercivity enhancement of grain-boundary-diffusion-processed Tb-treated Nd-Fe-B sintered magnets beyond the core-shell formation mechanism, where we determined the ultimate Tb concentration responsible for a significant (30 %) coercivity increase, that we published in the *Journal of Alloys and compounds (IF=4.65)*. The obtained results pave the way for engineering studies on grain boundaries that can be used to increase the coercivity of Nd-Fe-B magnets for e-mobility and green energy.

We have developed a new approach to the manufacture of Nd-Fe-B-type sintered magnets. The sintering process (pulsed electric current sintering PECS) is based on the rapid consolidation of magnetic powders into bulk metallic bodies by means of Joule heating. Short processing times, of the order of minutes, prevent extensive grain growth during sintering, potentially leading to improved magnetic performance. To reduce the use of critical heavy-rare-earth elements, a multicomponent magnet containing regions with different chemical compositions was prepared by adopting the already mentioned rapid sintering approach. Furthermore, we used the PECS method to produce hotdeformed Nd-Fe-B magnets with applicable magnetic properties, i.e., a coercivity of 1327 kAm^{-1}, a remanent magnetization of 1.27 T and a maximum energy product of 310 kJm^{-3} at a low sintering temperature and times. The results were published in the *Journal of Magnetism and Magnetic Materials (IF=2.717)* in three papers.

In 2020 we started with a new project under the frame of EIT RawMaterials, initiated and funded by the European Institute of Innovation & Technology (EIT); the **INSPIRES project** (INtelligent and Sustainable Processing of Innovative Rare-Earth magnetS), which 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. INSPIRES will optimize methods at an industrial scale for the sustainable extraction and recycling and use of recycled magnets in new motors.

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 to demonstrate the effective reuse of recycled rare-earth materials within several industries. The multidisciplinary SUSMAGPRO consortium are 20 of Europe's industry and academic leaders in REEs, sustainable processing, reuse, recycling, and recovery schemes, and cover the whole value chain from the collectors of magnet-containing scrap, to the producers of high-tech products.

As the coordinators, we continued with the European project **MaXycle** (A novel circular economy for sustainable REE-based magnets), a transnational collaborative research and innovation project, funded from the ERA-NET Cofund on Raw Materials (ERA-MIN 2) instrument under Horizon 2020. Already, first results showed that recycling EOL magnets would be a challenging task, as the difference in composition and coatings makes it impossible to develop a uniform recycling route. EOL magnets with no history are the most problematic as they have to be analyzed before recycling. That is why MaXycle is proposing a uniform labeling system for magnets for easy recyclability.

We successfully concluded two research and development projects for Kolektor d.d., Slovenian producer of bonded magnets based on Nd-Fe-B: (i) the improvement of the coercivity of melt-spun powders used for bonded magnets, and (ii) the development of a coating procedure using different coating materials to prevent corrosion in aggressive conditions. We successfully increased the coercivity by more than 15%, and we established so far, the most effective solution to protect sensitive Nd-Fe-B powders by using an optimized, thin protective layer. The improvement of coercivity was achieved by the addition of a Nd-Cu low-melting-point alloy, which was subsequently subjected to the optimized thermal treatment procedure. The upscaling potential of this technology was successfully verified by preparing 6 kg of coated powder for the pilot-plant production test. The results are excellent and will be further transferred to large-scale production. The final analyses showed that coated magnetic powder showed almost no loss of magnetic properties after 2 months of the aggressive corrosion test in demineralized water at 85 °C. The resistivity against corrosion of compressed bonded magnets was significantly improved, and the surface hardness of coated magnetic powders is lower than that of uncoated samples. This implies that the proposed powder-protection technology will not significantly change the existing tool wear used for the fabrication of final bonded magnets. This innovative approach is under protection with a patent application.

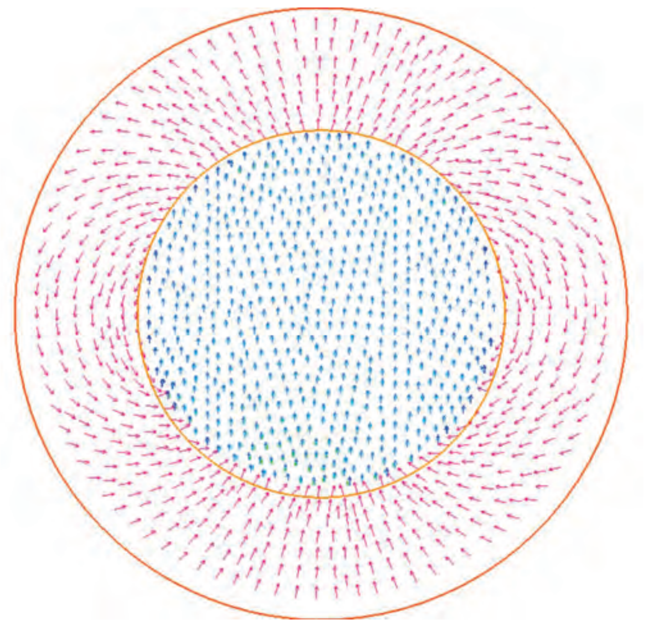

Figure 1: Calculated magnetization profile (red) for a Haalbach cylinder, with a homogenous magnetic field inside. A comparison between the prescribed (blue) and calculated (green) pattern.

Figure 2: 3D printed magnets produced by fused-filament fabrication. The particles were orientated during the printing with an external magnetic field.

We continued with 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 company Magneti Ljubljana, where we are investigating novel recycling of magnetic swarf based on Sm-Co. We found that the magnetic swarf can be fully recycled via re-melting technologies.

Additive-manufacturing technologies make it possible to produce magnets of arbitrary shapes and magnetization distributions. In order to design a magnet as the source of a given magnetic-flux field, expressed in terms of the lines-of-force pattern, it is necessary to solve the so-called magnetostatic inverse problem. With this aim we apply the adjoint-state and finite-element methods (figure 1).

In the frame of the ARRS project Development of complex shape multicomponent permanent magnets with the use of advanced 3D printing technology we are developing complex-shape, multicomponent, permanent magnets by additive manufacturing for the company Kolektor d.d. The goal is to increase the output of an electric motor using new magnet designs and multi-material usage in a single magnet. This complex shape will be printed with a state-of-the-art fused-filament fabrication method. In the first year we tested different polymers and magnetic powders to get the best filling factor that could still be printed (Figure 2). We successfully printed magnetic materials of different sizes and compositions. The next step is to print magnetic parts with orientated particles and to use debinding and sintering to produce fully dense, metal, 3D printed parts. The first tests on orientating the particles while printing showed promising results.

In 2020 we finalised the successful execution of the European project **AMPHIBIAN** (AnisoMetric Permanent HybrId magnets Based on Inexpensive And Non-critical materials) by closing the administrative work (reports) and consolidating manuscripts related to project's research activities. Two research and one review manuscripts were submitted to the *Journal of Physics D: Applied Physics (IF= 3.169)* (two accepted and one under review).

In parallel to the research framework of AMPHIBIAN, research activities in the field of possible strengthening of ferrite-based ceramic magnets were also initiated. Here, our research path is following the successful method of strengthening engineering ceramics using cellulose nanofibers (CNF) developed in collaboration with colleagues from Materials Science Institute (CSIC) of Madrid. Since consolidation is one of the important steps in the preparation of sintered magnets, different possibilities of how to prepare dense ferrite-based magnets were also explored. One of the emerging consolidation techniques that proved successful is sintering by intense thermal radiation (SITR).

Complex Intermetallic Alloys

In the frame of the International Research Laboratory, which was this year restructured into the International Research Project IRP PAC_2 "Push-Pull AlloyS and Complex CompoundS: from bulk properties to surface functions" we continued research in the field of Push-Pull alloys, which are part of complex metallic alloys (CMAs), with the emphasis on their preparation, properties and potential applications.

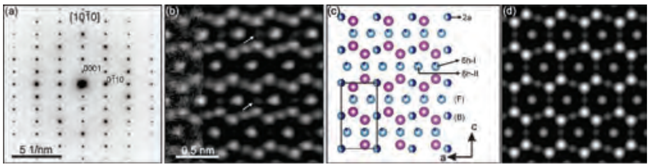

Figure 3: TEM studies of the ternary Laves phase: (a) SAED pattern analysis with the corresponding (b) atomically-resolved HAADF–STEM image. (c) Projected atomic model of the ternary Laves phase, viewed in $[10\bar{1}0]$ zone-axis with the related (d) calculated HAADF-STEM image.

We studied the Al-Cr-Sc ternary system, which has potential as a high-strength master alloy, with good thermal stability and corrosion resistance. We successfully synthesized a ternary Al-Cr-Sc phase, which belongs to the Laves phase group, prototype $MgZn_2$, and has a hexagonal crystal structure P63/mmc, space group 194 with a stoichiometry of $Al_{6.4}Cr_{1.6}Sc_4$. The crystal-structure refinement of the newly discovered phase showed a certain solubility range, which was further investigated by means of high-angle annular dark-field scanning-transmission electron microscopy (HAADF–STEM) combined with image simulations to quantify the observed intensity variations as a function of the mixed occupancies as predicted by the structural model (Figure 3).

Within the frame of low-adhesive, high-strength composite materials our main research was focused on a polymer matrix reinforced with an Al-Cu-Fe-B quasicrystalline powder. The main goal of this research is the development of a low-adhesive, high-strength composite material made of quasicrystals (QCs) and polymer polyphtalamide (PPA), which can effectively prevent future failures due to tribology problems, such as high-friction, fretting and cold welding. QCs have a low surface energy, low coefficient of friction, high hardness, good oxidation and corrosion resistance, low thermal and electrical conductivity, high wear resistance, non-stick properties, reduced wetting, but are brittle at room temperature. PPA belongs to the high-temperature engineering plastics and is chemically resistant, ductile, toughened, heat stabilized, has a high impact at low temperature and low warpage. First preliminary studies showed that the addition of QCs has a direct impact on the linear increase of maximum stress of the composite materials. In addition, a study of the Vickers hardness of different composite materials showed that a relatively low amount of QCs added to the polymer matrix does not have a significant influence on the overall Vickers hardness, but becomes significant when larger amounts of QCs are added to the system, for example 20 vol.% of QCs.

Structural Materials

As part of the ongoing long-term EUROfusion's European fusion program, we continued our research of the tungsten-carbide composites (W-W_2C) and binder-less tungsten carbide (WC) for the DEMO demonstration fusion power plant. The composition and the process of preparation of the W-W_2C composite materials were optimized based on a study of the interdependent relationships between the initial and final composition of the material directly affecting its temperature-dependent (room temperature 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 high-heat-fluxes testing (HHFT).

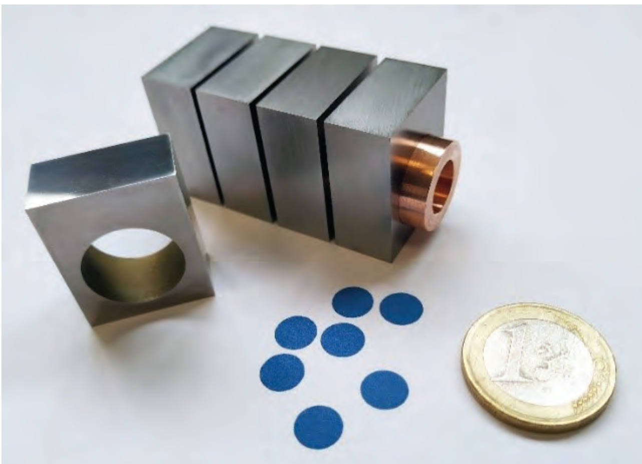
Figure 4: W-11WC monoblock components fabricated by spark-plasma sintering and shaped by electrical discharge machining

Based on the promising thermo-mechanical properties and HHFT determined in the previous 2019 campaign, the W-11WC composition (Figure 4) was selected for the fabrication of monoblock components, which were successfully produced and shaped to the specified dimensions. The samples will be joined to a CuCrZr cooling structure and subjected to HHF tests in an actively cooled mockup divertor system.

Sensors

In the field of HCHO electrocatalytic detection in alkaline media, we have fabricated KOH-modified, Ni-based receptor elements with different morphologies, surface chemical and crystal structures, and shape and dimensionality (i.e., 1D nanowires and 2D thin films). We investigated their electro-catalytic activity towards HCHO oxidation and elucidated the mechanisms for each individual Ni-based receptor element. The results of these studies were published in a highly ranked journals *Applied Surface Science (IF = 6.182)* and *Eletrochimica Acta (IF = 6.126).* The before-mentioned fundamental studies have shown that the HCHO oxidation in alkaline media is the most effective when using Ni nanowires. Hence, Ni nanowires have proven to be a promising and suitable candidate for use in a particular application or field of use. We developed a fully functional, Ni-nanowires-based sensor platform with Wi-Fi technology in collaboration with an electrical engineering expert. By testing the sensor platform, we detected HCHO in alkaline media, either in deionized or tap water. In recognition of this fundamental and applied research, the researcher Dr Špela Trafela was awarded by **L'Oréal-UNESCO National Programme for Women in Science in 2020**.

We are developing novel biosensing platforms (Figure 5) with high selectivity and specificity for the rapid detection of SARS-CoV-2 and its mutants in saliva samples. The fabrication of biosensing platforms will not be limited merely to SARS-CoV-2, but could be easily upgraded to detect different pathogens, and thus prevent the spread of future similar infectious disease.

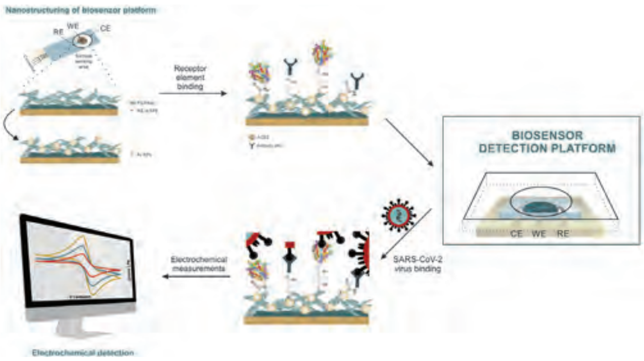

Figure 5: Schematic representation of SARS-CoV-2 detection using the electrochemical biosensor platform

We are developing receptor elements for the detection of toxic organic substances such as formaldehyde (HCHO) (national project L2-8182), acrylamide (AA) (national project J2-1739) and benzenediols.

Polyaniline is a conductive polymer with chemiresistive properties, which make it a widely used material for sensors. Polyaniline is studied for the potential resistivity sensing of gases like ammonia. We supplemented our fundamental electrochemical deposition studies by in-situ dynamic correlative approaches combining UV-vis spectroscopy and electrochemistry (spectro-electrochemistry) to understand the polymerisation mechanism in detail. The results were published in *The Journal of the Electrochemical Society (IF= 3.721).* In collaboration with the Department of Atmospheric Science and Environmental Engineering (Mines-Télécom Institute (IMT)) in Douai France, we have successfully combined our electrochemical system (electrochemically polymerized PANI on screen-printed electrode) with their knowledge of gas detection through resistance measurements. The result of the work is a feasible and direct construction of the NH_3 sensor from a PANI-screen-printed electrode, converted into a two-electrode system suitable for resistance measurements. We studied the responses to moisture, its stability, and the detection of the presence of NH_3 at 70% relative humidity. Despite a relatively simple system, without the presence of complex additives and nanomaterials, we achieved a low detection limit (23 ppb). The results of the collaboration are published in an article in *Sensors (IF=3.275).*

A new area of research is focused on the development of receptor elements for the selective and sensitive detection of benzenediols, namely catechol, resorcinol and hydroquinone. The sensor development paves the way to a portable and miniaturized sensor able to detect analyte in water and in the future also in air.

Materials for Health and a Clean Environment

In collaboration with the Queen's University Belfast, United Kingdom, and the Faculty of Medicine, University of Ljubljana, we have developed **temperature-sensitive liposomes** for immune- and chemo therapy and MRI-guided drug delivery. We investigated the effect of a PD1 blockade on the therapeutic efficacy of novel doxorubicin-loaded temperature-sensitive liposomes. The cytotoxicity of our nanocarriers and photothermally activated drug release were evaluated *in vitro*. Then, *in vivo* drug release and tumour accumulation of the nanocarriers was assessed using fluorescence and MRI, respectively. Finally, the therapeutic efficacy of a PD1 blockade in combination with photothermally activated drug-loaded magneto-liposomes in a CT26-tumour model was evaluated by monitoring tumour growth, cytokine release and immune cell infiltration in the tumour tissue. Doxorubicin therapeutic efficacy was potentiated in combination with anti-PD1 monoclonal antibodies, resulting in a significant reduction in CT26 tumour 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. This study is currently in the second round of revision in *Journal of Controlled Release (IF=7.870).*

As well as the field of cancer treatment, important results were achieved in diagnostics. The majority of the clinically approved iron oxide nanoparticles (IO NPs) used as **contrast agents for magnetic resonance imaging (MRI)** have been withdrawn from the market, either due to safety concerns or lack of profits. Therefore, there is a need for novel IO NPs-based imaging agents with a high safety margin and superior MRI properties. Thus, we investigated magnetic-liposomes with different formulations and tested their contrast performance for MRI. We found that the encapsulation of NPs into liposomes dramatically improves their contrast performance (up to 42-fold) due to the favourable interactions between the water visualized in MRI and the lipid coating. Importantly, an *in vitro* study showed improved selectivity of the magnetic-liposomes compared to the free nanoparticles. The cancer cells internalized a high concentration of liposomes, while their content was minimal in the normal cells, which led to an improvement in the contrast and an easier distinction between the healthy and the cancerous cells (Figure 7). In the case of free nanoparticles, the rate of internalization in both types of cell lines is similar and thus the diagnostics is limited. This study was published in *Nanomaterials (IF=4.324).* In addition, a review paper entitled "A Review on the Optimal Design of Magnetic Nanoparticle-Based T2 MRI Contrast Agents" was published in *Magnetochemistry (IF=1.947)*, where the factors affording r2 enhancement of magnetic nanoparticles were discussed (Figure 6).

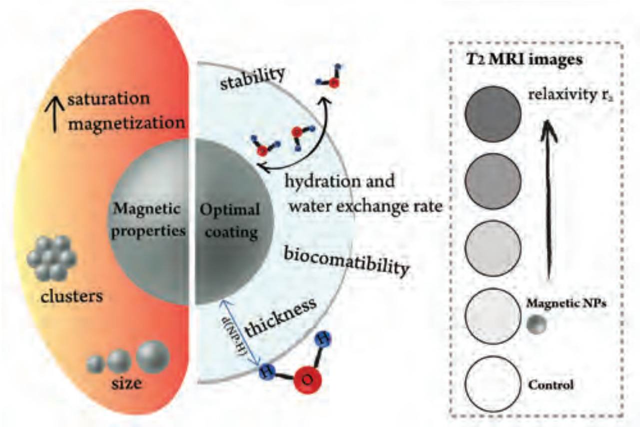

Figure 6: Relaxivity r_2 and thus the contrast efficacy of superparamagnetic nanoparticles (NPs) as MRI contrast agents can be enhanced via either the NPs' magnetic properties or coating optimization.

In collaboration with the Faculty of Health Science, University of Ljubljana, we have studied the adhesion specifics of pathogens that we performed, focused on the materials used for kitchen appliances, as well as specialized multi-layer coatings that either destroy or limit the adhesion of the bacteria. *E. coli, P. aeruginosa* and *C. jejuni* have been chosen as test bacteria as they are the most common food-borne contaminants that adhere to kitchen surfaces (ceramics, Teflon). The hydrophobic nature of Teflon proved to be the decisive factor that determines bacterial adhesion (*International journal of food microbiology, IF=3.451).* A study we published in *Biofouling (IF=2.351)* paired bacterial adhesion against differently mechanically treated steel substrates. It was shown that surface asperities predominantly affect the bacterial attachment point and its ability to grow a biofilm. Moreover, we evaluated dishwashing and the misuse of the detergent that led to elevated amounts of residues on the dishes and may cause long-term side effects on our health and environment, published in *Environmental chemistry letters (IF=5.849).* Finally, we evaluated the bacterial adhesion capacity of protein-terminating polyelectrolyte multilayers and it was shown that in the case of a lysozyme-terminating layer the lysis takes place, whereas in the case of BSA and glucanase-specific protein-bacteria interactions are dominant (Figure 7). The study was published in the *International journal of adhesion and adhesives (IF= 2.671).*

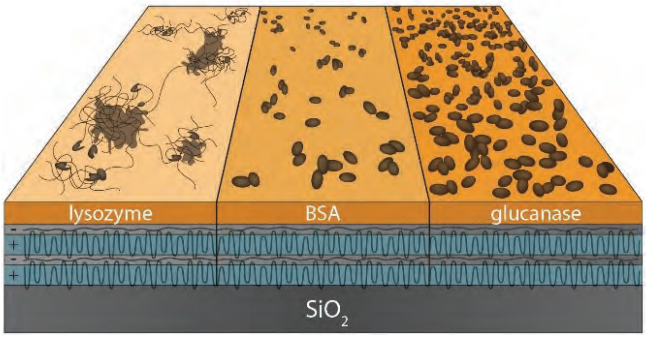

Figure 7: Schematic presentation of bacterial adhesion on protein-terminating polyelectrolyte multilayers with lysozyme, BSA and glucanase as final layers.

The final goal of the ongoing study within the ARRS project Degradation of textile microplastic for domestic wastewater treatment is to eliminate microplastic fibers released from common washing machines' drains through degradation processes, such that when released it will be harmless and ecologically unproblematic. A TiO_2 photocatalyst was used for the photocatalytic degradation of microplastics, which has proved to be successful, but the studies are still in the initial phase of the research. The obtained results showed that individual PP fibers were not as smooth as the pristine fibers. PET fibers delaminated and deformed, while PA fibers thinned by almost 50 percent, which indicates that the degradation strongly effects the surface proven with environmental scanning electron microscopy (ESEM). We have also found chemical changes using Raman spectroscopy. The first successful trials were made and explained in detail on Water days 2020 and the 5th Green and Sustainable Chemistry Conference. Within the scope of an ongoing collaboration with the UL Biotechnical faculty within the ARRS project Degradation of plastics with polyextremotolerant fungi, we showed that certain types of fungi, for example, *Pleurostoma sp*. and *Coniochaeta sp*., grow on pristine plastic fibers, utilizing the plastic as the sole source of carbon in our growth medium (Figure 8).

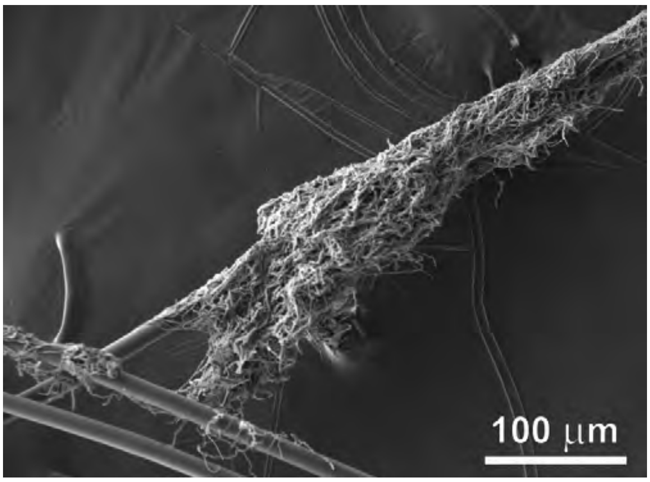

Figure 8: PET fibres overgrown with Coniochaeta sp.

Biomaterials

As a partner in an ARRS funded project that is being carried out in collaboration with the Faculty of Veterinary Medicine, University of Ljubljana, we continued our research on the silk fibroin carrier for hormone release. The 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 *in vivo* animal testing of the first fibroin films started. Knowledge of the processing of various biomaterial-based carriers and scaffolds will be used in a newly granted ARRS project, entitled *Advanced 3D cell models: Bridging the gap between in vitro and in vivo experimental systems (hep-3DGenTox)*, that will be conducted in collaboration with Department of Genetic Toxicology and Cancer Biology of the National Institute of Biology (lead party).

The past knowledge of the biomaterial group on bioactive glasses and other calcium-silicate cements has been successfully exploited under the framework of a granted ARRS project, entitled Post-radiation caries in head and neck cancer patients: Aetiology and prevention, conducted in collaboration with the University Medical Centre Ljubljana (lead party). The project aims to understand the mechanism of the formation of deep caries lesions in patients being cancer treated by radiation. In addition, by understanding the cause of physiochemical changes in the inorganic and organic parts of the tooth a prevention and treatments to reverse the carries formation a Ca-silicate based formulation are being developed.

Catalysis

In the field of **photo-electro-catalysis**, we continued research on the anodization process of flexible titanium foils and factors influencing the growth of rigidly attached TiO_2 nanotubes. On six different thicknesses of anodized titanium foils, we investigated the photocatalytic activity, adhesion of TiO_2 nanotubes, and the influence of electrolyte age on the growth and catalytic properties of TiO_2 nanotubes. We have successfully identified the main experimental parameters that enable the growth of a flexible catalyst that can be used to purify organic pollutants from water and air.

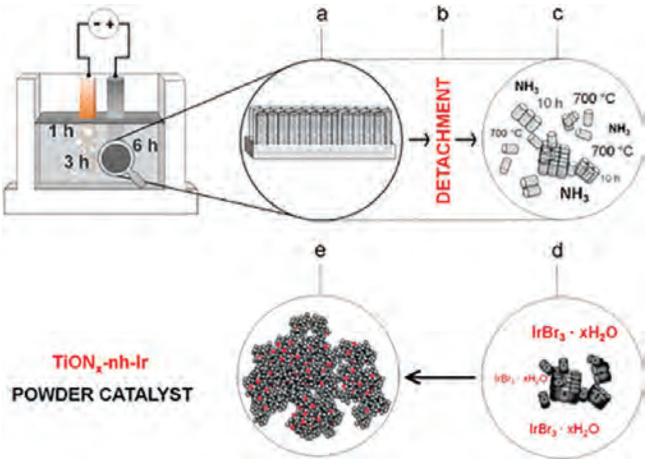

Figure 9: Procedure for $TiON_x$-nh-Ir catalyst preparation. (a) Anodic oxidation of titanium foil, (b) detachment of TiO_2 nanotubes, (c) annealing of detached TiO_2 nanotubes in ammonia, (d) deposition of Ir onto $TiON_x$ nanotubes, and (e) the final $TiON_x$-nh-Ir powder catalyst.

With the National Institute of Chemistry we collaborated in two studies, where TiO_2 nanotubes were prepared by anodic oxidation and subsequently treated in ammonia at elevated temperature. The process resulted in a TiO_xN_y substrate with a large surface area of the immobilized film and/or powder. Afterwards, Ir nanoparticles (Figure 9) were applied to the substrate or to the powder and the efficiency of the catalysts for electrocatalytic water splitting were investigated. The results showed the very high activity and stability of both catalysts for the oxygen evolution reaction (OER) in an acidic medium. These outstanding studies were published in two separate scientific papers in *ACS Catalysis (IF=12.350)*.

Towards the end of the research year, we designed a project of ***Automated laboratory*** for the autonomous research of new materials. Within this project, we will implement robotized experimental and analytical procedures that will enable us to carry out practical experiments much more reliably, traceably and faster, thus eliminating the main disadvantages and deficiencies of standard materials-processing approaches. Consequently, the implementation of this new approach in the synthesis and processing of materials will enable us to have a more efficient and insightful interpretation of the experimental data.

Engineering Ceramics

The naturally self-driven AlN powder hydrolysis was exploited for a quick, facile and pure synthesis path for the preparation of abundant amounts of hierarchically assembled, nanocrystalline, mesoporous alumina (MA) powder in the form of micron-sized bundles of agglomerated nanocrystalline 2D lamellas, or nanosheets, forming flower-like structures. A part of a PhD project included a study of the dispersion and rheological behaviour of aqueous suspensions containing MA powder. The aim was to prepare suspensions, containing micron-sized particles of γ–Al_2O_3, able to defy sedimentation and segregation. The addition of divalent cations (Mg^{2+} in Ca^{2+}) or cellulose nanofibers (CNF) triggered the formation of various interparticle associations for tailoring the sedimentation and the stability of these suspensions (Figure 10). The work was published in the leading scientific journal for ceramic materials *Journal of the European Ceramic Society (IF=4.495)*. Preparation of such suspensions is an important milestone in the preparation of advanced, porous ceramic materials relevant to catalysis and adsorption.

The AlN-powder-hydrolysis-derived hierarchical MA structures were adopted in a study published in the renowned scientific journal *Green Chemistry (IF= 9.480)*, in collaboration with the Department for Materials Synthesis (JSI) and the Department of Catalysis and Reaction Engineering of the National Institute of Chemistry. The paper demonstrates the application of a magnetic heating of nanoparticles in an AC field to drive a substantially more efficient chemical reaction/conversion of furfural to furfuryl alcohol over the catalyst as compared to conventional reactor heating.

In the field of dental ceramics, we have traditionally been involved in the research of zirconia dental ceramics. In 2020, we have finalised a study in collaboration with start-up company Vall-cer d.o.o., where we have evaluated the effect of continuous impacting between zirconia (3Y-TZP) dental root posts during 500-hour-long shaking on the extent of (sub) surface microstructural changes affecting the fracture strength. With an increase of the shaking time the surface roughness decreased, where the grains were flattened and partially spalled. The observed 6-micrometre-thick altered subsurface region containing compressive residual stresses contributed to a systematic increase in the forces of fracture within the sample population; however, only for those containing the surface type of critical flaws that were in the form of mould imprints. The work was published in *Journal of the European Ceramic Society (IF=4.495).*

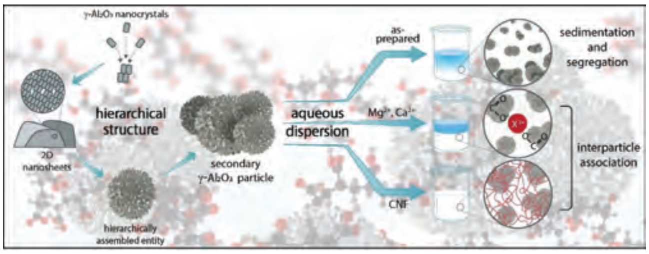

Figure 10: Illustration of the proposed mechanism of hierarchical assembly of γ-Al_2O_3 nanocrystals to MA particles and an overview of the implemented mechanisms against sedimentation and segregation.

Functional ceramics: semiconducting ZnO-based ceramics (varistors, thermoelectrics)

In the field of oxide thermoelectric materials, we continued with the development of the n-type ZnO-based ceramics for energy-harvesting applications at medium and high temperatures. The focus of the research is the influence of interfaces like grain boundaries and special planar defects (i.e., inversion boundaries) on charge and heat transport. Understanding of these phenomena is essential to enhance the electrical conductivity (σ), while preserving the high Seebeck coefficient (S) and to reduce the thermal conductivity. The aim is bottom-up structural and microstructural engineering of ZnO-based ceramics with significantly improved thermoelectric properties. Accordingly, the influence of the starting ZnO powder doped with selected elements like Al, In and Co in very low amounts of few at.% and sintering methods on the thermoelectric characteristics was studied. We collaborated with the National Institute for Materials Science (NIMS, Tsukuba, Japan) in the study, which showed that the powder of Al-doped porous aggregates of ZnO nanoparticles enable the preparation of the ZnO ceramics with substantially enhanced thermoelectric characteristics. The ZnO nanopowder was synthesized by a novel and simple interface-reaction method (double-emulsion method). Densification of such powder using SPS results in ceramics with markedly suppressed lattice thermal conductivity due to a significant reduction of the ZnO grain size, inclusions of fine Al-rich nanoparticles and nanoporosity. Also, electrical conductivity (σ) and power factor (PF = sS^2) are enhanced by increased donor (Al^{3+}) doping of the grains. In collaboration with NIMS we continued with our research about the influence of doping with magnetic elements such as Co on the structural, microstructural and thermoelectric properties of the Al-doped ZnO ceramics. The results showed that the electrical conductivity and the power factor of the ceramics are increased for about 50% already with the addition of 0.25at.% of Co. Additions up to 0.5 at.% Co increase the thermal conductivity, but with higher additions it decreases. Furthermore, within collaboration with the CRISMAT Laboratory (Caen, France) we started to study the influence of using either fine ZnO nanopowder with a particle size of about 20–30 nm or coarser ZnO powder with a particle size of about 200 nm on the microstructure development and thermoelectric characteristics of the ZnO ceramics doped with up to 4 at.% of Al and up to 1.5% of In.

In collaboration with the Shanghai Institute of Ceramics, Chinese Academy of Science – SICCAS we continued studies of the ZnO ceramics with specific electrical characteristics. Our previous studies showed that classic sintering in a reducing atmosphere and also spark-plasma sintering (SPS) in a vacuum prevent the formation of electrostatic Schottky barriers at the grain boundaries and strongly increase the solid solubility of donor dopants such as Al in the ZnO grains. Consequently, increased charge-carrier concentration and mobility result in several orders of magnitude higher electrical conductivity (σ), while increasingly the defect structure due to a large concentration of point defects reduce the lattice conductivity significantly. Further studies also showed that although annealing of such ceramics in air results in strongly reduced electrical conductivity and hence also power factor due to the formation of Schottky barriers at the grain boundaries, their power factor is still 8-times higher than in ceramics prepared only by sintering in air. Results confirmed the advantages of such two-stage sintering of the ZnO-based ceramics for the thermoelectric applications. Accordingly, studies were aimed to evaluate the influence of annealing in air on an eventual decrease of the Al solid solubility in ZnO and its precipitation in grains or at the grain boundaries, degree of structural defectness, changes in the microstructure and consequently the thermal conductivity of ceramics conventionally sintered under a reducing atmosphere or SPS in vacuum. With SICCAS we also continued the research on the development of the new type of the ZnO-based varistor ceramic with a very simple chemical composition and without standard varistor dopants like oxides of Bi_2O_3 (problem of liquid phase formation and evaporation during sintering), Pr (expensive) and others (Ni, Cr).

Collaboration with company Bourns is aimed to enhance the current-voltage (I-U) characteristics and stability of the ZnO-based multilayer varistors. In collaboration with the Faculty of Mechanical Engineering, University of Ljubljana and the VARSI company we study the influence of the surface machining of ceramics on their performance.

Mineralogy

A newly initiated collaboration with the Department for Litospheric Research of Vienna University in the frame of FWF-ARRS International Project GInA: 'Mineral inclusions in garnets from macroscopic to atomic scale – opening the petrogenetic archive' and FWF-RFBR International Joint Project MiMa: 'Fe-Ti oxide inclusions and magnetism of oceanic gabbro' was dedicated to experimental studies of petrological samples. The planned visits were stringently reduced due to the COVID-19 outbreak and the research was conducted with minimum interactions. Except the kickoff meeting in January, all further project meetings were held on-line. Collaboration with Dr. Pavel N. Gavryushkin from the University in Novosibirsk was strengthened and connected to the existing collaboration with Acad. Prof. Mihály Pósfai from the University of Veszprém. Trilateral collaboration aims to address **the theoretical and structural aspects of the aragonite problem**.

Self–assembly: Our studies were focused on the unusual displacements of rutile fibers grown on rutile templates that could not be explained by simple epitaxial growth. For this purpose, we prepared models for virtual ab-initio experiments aimed to resolve this problem. On the pure surfaces the optimization did not converge at all, and the fiber separation was too large for hydrogen bonding, therefore we designed models with hydrated interface, which closely simulate experimental conditions. DFT optimization showed an interesting trend of protonation in the case of shift, which was not present in the models with no shift, directly suggesting that the observed displacements are generated by acidic medium. Our studies give a **fundamental insight into self-assembly processes on the atomic scale.**

Semiconductors: Collaboration with Dr. Ildiko Cora from the Institute of Technical Physics and Materials Science of the Hungarian Academy of Sciences in Budapest on **in-situ TEM studies** of the Ga_2O_3 transformation resulted in a highly ranking, joint publication in *Acta Materialia (IF= 7.656).* The work was conducted as a part of Slovenian–Hungarian bilateral project (Characterization of structural defects in semiconductor ZnO films grown by atomic layer deposition (ALD)). Quantum chemical and high-resolution TEM studies of stability and the formation of chemically induced planar defects in crystals done in a collaboration with the Institute for Multidisciplinary Research in Belgrade resulted in another excellent publication in *Acta Materialia (IF= 7.656).* We demonstrated that **ab-initio calculations can be used as a powerful tool to perform virtual experiments that have the capacity to predict and to reproduce experimentally observed non-periodic features, such as interfaces**, which are responsible for the quantum properties of materials. Combining atomistic modeling, DFT calculations and HRTEM analysis we provided a new, fundamental insight into the structure and stability of Sb-rich, basal-plane IBs in ZnO. DFT screening for the most stable IB model had an unexpected outcome – it predicted a model that was previously not known in this system, to be the most stable one, and that the generally accepted IB model, identified by our group in 2001, is the second most stable. This surprising result was verified by careful HRTEM screening of Sb_2O_3-doped ZnO samples that resulted in an experimental confirmation of the theoretically identified structure. We showed that the energies of the constituting stacking segments can be used to predict the stability of IB structures without the need for further ab-initio calculations (Figure 11). Our study demonstrates that the quantum-chemical modeling of materials can be leveraged with atomic-scale electron microscopy methods to extract fine structural details from interfaces. Refined structures are fundamental to solving the open questions related to their role in the electron transport, phonon scattering, the mysterious p-type conductivity of ZnO, the affinity of dopants to generate IBs and the underlying formation mechanisms, whereas the excellent match between the calculations and experiment demonstrated in our study opens new perspectives for the prediction of such properties from first principles. Linking the two faces of the phenomenon, our study makes a bridge between two scientific communities both working at the atomic scale, theoreticians and experimentalists, and will inspire these complementary groups to work hand in hand at solving fundamental materials science problems.

Studies of microstructure evolution and electrical properties of SnO_2-based varistor ceramics were concluded by publishing two further papers in the Journal of the European Ceramic Society (IF=4.495).

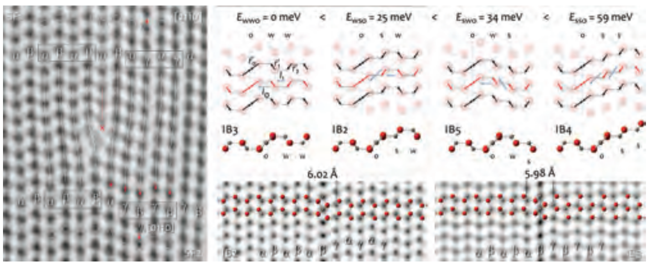

Figure 11: SFs as a preparatory stage of IB formation (left). DFT analysis of possible stacking modes demonstrates that a thermodynamically more stable structures involve fewer cubic bonds (above). The two stable IB structures in Sb_2O_3-doped ZnO: the old one (IB_2) known from quantitative HRTEM study of IBs by Rečnik et al. (2001), and the new, more stable IB structure (IB_3), predicted by DFT screening. Both IB structures coexist and are confirmed experimentally (published by Ribić et al. Acta Materialia (2020)).

Advanced Electron Microscopy

For the microstructural characterization of materials we use advanced **correlative microscopy**, which means the application of combined and optimized several analytical microscopic methods including: scanning electron microscopy (**SEM/FEGSEM**), qualitative and quantitative elemental analysis by electron-probe microanalysis (**EPMA**) with energy-dispersive (**EDXS**) and wavelength-dispersive (**WDXS**) X-ray spectroscopy, electron-backscatter diffraction (**EBSD**) and complementary light optical microscopy (**LOM**) and atomic force microscopy (**AFM**) (Figure 12).

By using optimized correlative microscopy, we have studied various materials such as: thermoelectric ceramics, varistor ceramics, complex metallic alloys and quasicrystals, permanent magnetic materials based on Nd-Fe-B and Sm-Fe-Co, abrasives.

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

The research group of the Department for Nanostructured Materials is very 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 research infrastructure for electron microscopy.

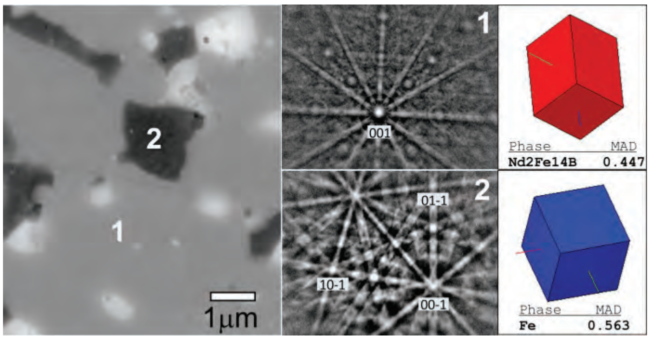

Figure 12: Correlative FEGSEM-EBSD microanalysis of the Nd-Fe-B material with the marked matrix phase $Nd_2Fe_{14}B$ (1) and secondary α-Fe phase (2) with the corresponding EBSD patterns, unit-cell orientations and phase identification.

ESTEEM consortium, which was successfully granted its third ESTEEM INFRAIA project (ESTEEM3), has the status of an EU Advanced Community. A member of our department is the coordinator for networking activities (NAs) within the project.

Industrial partners

Within the project "*Microstructural investigations of abrasive materials*" with industrial partner *Weiler* Abrasives*, Zreče* we have investigated innovative composite abrasives, intended to develop and manufacture improved cutting and grinding tools with a prolonged lifetime.

Education and outreach activities

For the eighth year, the members of the department participated in science promotion activities within the framework of the Science on the Street project. We organized 13 live and virtual popular-science lectures. On the ZnC website we have published 5 blogs of researchers and 2 contests. At the invitation of the EIT "Raw Materials" and JA Slovenia (Institute for the Promotion of Youth Entrepreneurship), we co-organised the Innovation Camp 2020. One hundred students from 20 high schools from all over Slovenia participated in the Innovation Camp.

The members of the department are further involved in the education program at the Jožef Stefan International Postgraduate School, Faculty of Natural Sciences and Engineering, UL and at the Academy of Fine Arts and Design, UL.

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 III. phase of SRIP ToP for the period 2020–2023 which is following the successful conclusion of the II. phase.

Awards and appointments

1. Dr Špela T**rafela** was awarded by L'Oréal-UNESCO National Programme for Women in Science in 2020 in recognition of her fundamental and applied research. She has developed nanostructured sensor platforms based on a $Ni(OH)_2$/NiOOH-Ni redox system for the electrochemical detection of formaldehyde in alkaline media.
2. After receiving the Krka Prize in 2019, for the study entitled "Colloidal silver in dental products", students Laura Drasler and Ula Dragman, from the Vič High School, under the mentorship of prof. Alenke Mozer (Vič High School) and **Anje Korent** (JSI, K7), submitted a research paper to the GENIUS Olympiad 2020 competition. The submitted research paper has made it to the finals of the GENIUS Olympiad 2020. The research focuses on a study of the colloidal silver concentration in dental products such as toothpaste, mouthwash and toothbrush. Commercial products with silver content were purchased and studied by students at the K7, IJS laboratories.

3. The Editorial Board from the prominent journal Green Chemistry selected a paper by **Xuan Xu**, **Sašo** Šturm, **Zoran Samardžija**, **Janez** Ščančar, **Janez**, **Katarina Marković**, **Kristina** Žužek **Rožman**, all from the Jožef Stefan Institute, entitled "A facile method for the simultaneous recovery of the rare-earth elements and transition metals from Nd-Fe-B magnets" as a 2020 HOT *Green Chemistry* **article**. The paper is a result of the ITN-MSCA project DEMETER, Training Network for the Design and Recycling of Rare–Earth Permanent Magnet Motors and Generators and Full Hybrid and Electric Vehicles [2015-2019] for which funding is gratefully acknowledged.
4. **Prof. Dr Sašo** Šturm, Head of Department for Nanostructured Materials, was elected as a member of the Executive Board of European Microscopy Society (EMS) in August 2020. The EMS is an umbrella organization that brings together all national microscopy societies. Prof. Dr Sašo Šturm was proposed by the Slovene Society for Microscopy (SDM) Executive Board and thus the Slovenian representative in the EMS Executive Board was elected for the first time.

Organization of conferences, congresses and meetings

1. Annual meeting of LIA PACS2: International Associated Laboratory; Push-Pull AlloyS and Complex Compounds: from bulk properties to surface functions, 5 November 2020 (co-organisers, virtual)
2. The 12th Jožef Stefan International Postgraduate School Students' Conference and 14th CMBE day, 15 May 2020 (co-organisers, virtual)

Patent granted

1. Paul J. McGuiness, Marko Soderžnik, Kristina Žagar, Andraž Kocjan, Spomenka Kobe, Method of manufacturing fully dense Nd-Fe-B magnets with enhanced coercivity and gradient microstructure, EP2869311 (B1), European Patent Office, 24. 06. 2020.

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. Spark Plasma Sintering (SPS) of Cost Effective and High Performance Rare-Earth Based Permanent Magnets for Electrical Machines
   Prof. Spomenka Kobe
   ABB Switzerland Ltd
3. COST CA17140 - Nano2Clinic; Cancer Nanomedicine - From the Bench to the Bedside
   Dr. Nina Kostevšek
   Cost Association Aisbl
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 - EUROfusion; Plasma Facing Components-1-IPH-FU, EUROfusion
   Prof. Saša Novak Krmpotič
   European Commission
7. H2020 - EUROfusion; Materials-PPPT-FU
   Prof. Saša Novak Krmpotič
   European Commission
8. H2020 - EUROfusion; Education-ED-FU
   Prof. Saša Novak Krmpotič
   European Commission
9. Investigation of Helium Retention in Plasma Facing Materials Using Advanced Analytical Methods
   Asst. Prof. Janez Zavašnik
   Slovenian Research Agency
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

RESEARCH PROGRAMMES

1. Nanostructured Materials
   Prof. Sašo Šturm
2. Ceramics and complementary materials for advanced engineering and biomedical applications
   Asst. 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
   Asst. 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. Catalytically-assisted high efficiency and low-cost nanostructured sensors based on modified screen printed electrodes for analytical chemistry
    Prof. Kristina Žužek Rožman
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
Dr. Kristina Žagar Soderžnik
15. Designing functionality of lead-free ferroelectrics through domain wall engineering
Asst. Prof. Matej Andrej Komelj
16. UV sensors nanoparticles embedded into PA fibres
Prof. Spomenka Kobe
17. Effective recycling of abrasive sludge in the production of Sm2Co17 magnets for a waste-free economy
Prof. Kristina Žužek Rožman
18. Development of complex shape multicomponent permanent magnets with the use of advanced 3D printing technology
Prof. Spomenka Kobe
19. Degradation of textile microplastic for domestic wastewater treatment
Dr. Matejka Podlogar
20. Novel Flow Photoelectrocatalytic Reactors for Degradation of Pharmaceuticals in Waste Water
Prof. Miran Čeh
21. Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF)
Dr. Kristina Žagar Soderžnik
Ministry of Economic Development and Technology
22. 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
23. A novel ciruclar economy for sustainable RE-based magnets
Prof. Spomenka Kobe
Ministry of Education, Science and Sport
24. Services for the Exports
Dr. Zoran Samardžija
25. External Services
Asst. Prof. Andraž Kocjan

NEW CONTRACTS

1. 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.
2. Novel Flow Photoelectrocatalytic Reactors for Degradation of Pharmaceuticals in WasteWater
Prof. Miran Čeh
Arhel Projektiranje in Inženiring d. o. o.
3. Characterization of surface structure of machined ceramic materials
Prof. Slavko Bernik
University of Ljubljana

VISITORS FROM ABROAD

1. Laia Alfonso, Marina Salord Fiol and Maria Fernandez, University of Barcelona, Barcelona, Spain, 16 September 2019 to 16 January 2020
2. Dr Vincent Fournee, Institut Jean Lamour, Nancy, France, 21–26 January 2020
3. Dr Gerlinde Habler, Ge Bian, Olga Ageeva, Taisia Alifirova, Victoria Kohn, Rainer Abart, Thomas Griffiths, University of Vienna, Vienna, Austria, 22–31 January 2020
4. Dr Miguel Bernal and Dr Jon Ustarroz, Université Libre de Bruxelles, Brussels, Belgium, 2–9 February 2020
5. Dr Goran Branković, University of Belgrade, Belgrade, Serbia, 11–14 February 2020
6. Dr Thomas Schrefl, Danube University Krems, Krems an der Donau, Austria, 13–14 February 2020
7. Prof. Stoja Rešković, Zavod za mehaničku metalurgiju, Sveučilište u Zagrebu, Metalurški fakultet, Sisak, Croatia, 24 February 2020
8. Büşra Günhan, Kütahya Dumlupınar University, Kütahya, Turkey, 14 January to 16 March 2020
9. Vesna Ribić, University of Belgrade, Belgrade, Serbia, 1 February to 31 December 2020
10. Dr Sophie Legeai, Institut Jean Lamour, University of Lorraine, France, 5–7 March 2020
11. Milan Vukšić, Fakultet strojarstva i brodogradnje u Zagrebu, Sveučilište u Zagrebu, Zagreb, Croatia, 1 March to 6 April 2020
12. doc. Dr Aleš Omerzu, Univerza v Rijeki, Rijeka, Croatia, 7 July 2020
13. Milan Vukšić, Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Croatia, 28 June–26 July 2020
14. Lana Staver, Faculty of Medicine, University of Ljubljana, Ljubljana, Slovenia, 5–7 August 2020
15. Andrea Delgado López, Gran Via de les Corts Catalanes, Barcelona, Spain, 1 October to 31 December 2020
16. Dr Richard Wheeler, Edinburgh Scientific, Edinburgh, Scotland, 3 September 2020
17. Tomaž Bojko and Dr Cy Su, Keko-Varicon družba za proizvodnjo in razvoj elektronskih Komponent, d.o.o., Žužemberk, Slovenia, 23 September 2020
18. Tina Zajc Benda, RIS Manager, EIT RawMaterials Innovation Hub CLC East Sp. z o. o, Wrocław, Poland, 14 October 2020

STAFF

Researchers
1. Prof. Slavko Bernik
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4. Dr. Aljaž Iveković
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7. Asst. 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. *Asst. Prof. Janez Zavašnik, 01.05.20, transferred to Department F6*
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20. Dr. Nataša Drnovšek*
21. *Dr. Vanja Jordan, left 23.11.20*
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23. Dr. Nina Kostevšek
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45. Dr. Boris Saje*

Technical and administrative staff
46. Darko Eterović
47. Tomislav Pustotnik

Note:
* part-time JSI member

BIBLIOGRAPHY

Original Article

1. Marjan Bele *et al.* (12 authors), "Increasing the oxygen-evolution reaction performance of nanotubular titanium oxynitride-supported Ir nanoparticles by a strong metal-support Interaction", *ACS catalysis*, 2020, **10**, 22, 13688-13700.
2. Darja Lisjak, Patricija Hribar, Alenka Mertelj, Andraž Mavrič, Matjaž Valant, Janez Kovač, Hermina Hudelja, Andraž Kocjan, Darko Makovec, "Formation of Fe(III)-phosphonate coatings on barium hexaferrite nanoplatelets for porous nanomagnets", *ACS omega*, 2020, **5**, 23, 14086-14095.
3. Tjaša Matjašič, Tanja Dreo, Zoran Samardžija, Oliver Bajt, Tjaša Kanduč, Tatjana Simčič, Nataša Mori, "Preliminary experiments into colonization of microorganisms from activated sludge on different types of plastics", *Acta biologica slovenica: ABS*, 2020, **63**, 1, 45-61.
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REVIEW ARTICLE

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PUBLISHED CONFERENCE CONTRIBUTION

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Patent Application

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Patent

1. Paul J. McGuiness, Marko Soderžnik, Kristina Žagar, Andraž Kocjan, Spomenka Kobe, *Method of manufacturing fully dense Nd-Fe-B magnets with enhanced coercivity and gradient microstructure*, EP2869311 (B1), European Patent Office, 24. 06. 2020.

Theses and Mentoring

1. Bojan Ambrožič, *In situ synthesis and growth of nanoparticles using a liquid cell transmission electron microscopy:* doctoral dissertation, Ljubljana, 2020 (mentor Sašo Šturm).
2. Sorour Semsari Parapari, *Fluorination of vanadium oxy-phosphates for high-energy cathode materials of li-ion batteries:* doctoral dissertation, Sabanci, 2020 (mentor Mehmet Ali Gulgun; co-mentor Robert Dominko).
3. Špela Trafela, *Development of nanostructured redox couple $Ni(OH)_2$ NiOOH-Ni based receptor elements for detection of formaldehyde in alkaline media:* doctoral dissertation, Ljubljana, 2020 (mentor Kristina Žužek Rožman).

DEPARTMENT FOR MATERIALS SYNTHESIS K-8

The research of the Department for Materials Synthesis is mainly related to the synthesis of various advanced materials, especially magnetic materials, semiconducting oxides and optical materials. Special attention is given to nanostructured materials, such as ferrofluids, functionalized nanoparticles for use in biomedicine, multifunctional nanocomposites, magnetic coatings and fluorescent nanoparticles.

Head:
Prof. Darko Makovec

A large part of the research at the Department for Materials Synthesis is devoted to the synthesis of nanoparticles. The wet-chemical synthesis of inorganic materials with complex compositions and crystal structures in the form of small nanoparticles has great potential for the discovery of new compounds. Namely, according to the empirical Ostwald step rule, metastable polymorphs frequently nucleate before the stable phase due to a lower nucleation barrier. These metastable polymorphs can be stabilized at the small size of the nanoparticles if the surface energy of the metastable phase is lower to that of the stable phase. The metastable polymorphs stabilized at the nanoscale represent some of the technologically most important nanomaterials, e.g., photocatalytic anatase and magnetic maghemite nanoparticles. Even through it is expected that such metastable polymorphs are not restricted to simple oxides, they were never reported for the mixed oxides with a complex structure. Our systematic research of mechanisms involved in the formation of two types of mixed oxides, magnetic hexaferrites ($AFe_{12}O_{19}$, A = Ba, Sr, Ca) and ferroelectric Aurivillius bismuth titanate ($Bi_4Ti_3O_{12}$) during their hydrothermal synthesis confirmed the immense potential of the stabilization of new metastable polymorphs for the discovery of new nanomaterials.

The hydrothermal synthesis of hexaferrite nanoplatelets has been a topic of our research for decades. The barium-hexaferrite nanoplatelets exhibit unique magnetic properties defined by their very large, uniaxial magnetic anisotropy, with the easy axis perpendicular to the platelet. They already enabled the development of new materials, e.g., ferromagnetic fluids, soft magneto-electrics, and magneto-optic composites. However, for applications in medicine, barium hexaferrite is not the preferred material because of the potential toxicity of barium. With the hydrothermal method we can also synthesize strontium-hexaferrite nanoplatelets; however, their magnetic properties cannot match those of the barium analogue. A systematic study of nanoplatelet formation using conventional methods (TEM, XRD) did not show any significant differences between the two analogues. Different mechanisms were only revealed by an analysis of the nanoplatelets' structure with an atomic-resolution scanning-transmission electron microscope (ARM). The Ba-hexaferrite forms in reactions between Ba- and Fe-hydroxides at temperatures below 80 °C as ultrafine, less-than-20-nm-wide discoid nanoplatelets. Their structure can be represented in terms of two alternating structural blocks: a hexagonal $(BaFe_6O_{11})^{2-}$ R block and a cubic $(Fe_6O_8)^{2+}$ spinel S block, as a SRS* segment of the hexagonal magnetoplumbite RSR*S* unit cell (S.G.: P63/mmc, a = 5.88 Å, c = 23.05 Å). With the exaggerated growth above 150 °C, the nanoplatelets' thicknesses increase discretely with the addition of the RS segments to their initial structure. Also, the Sr-hexaferrite forms as the ultrafine discoid nanoplatelets (2–5 nm thick and a few tens of nm wide); however, the ARM analysis showed that they have completely different structure than the Ba-hexaferrite nanoplatelets. They exhibit an incredibly complex crystalline structure with a very large hexagonal unit cell (a= 56.6 Å, c=18.0 Å) (Figure 1). With exaggerated growth above 160 °C, the discoid nanoplatelets with the new structure recrystallize into larger hexagonal nanoplatelets with the equilibrium magnetoplumbite structure. The new structure also transforms to the magnetoplumbite during heating at temperatures above 500 °C. The new structure clearly represents a metastable polymorph stabilized on the nanoscale. The difference in the development of the structure of two hexaferrite analogues was related to their thermodynamic stability. The stability of $AFe_{12}O_{19}$ hexaferrites decreases with a decreasing size of the A-ion: the Ba analogue is more stable than the Sr analogue, whereas the Ca analogue is only stable when partially substituted with larger ions (e.g., with a combination of La^{3+} and Co^{2+}). The influence of the thermodynamic stability of

Discovery of new polymorphs in mixed oxides with a complex crystal structure: strontium hexaferrite and bismuth titanate.

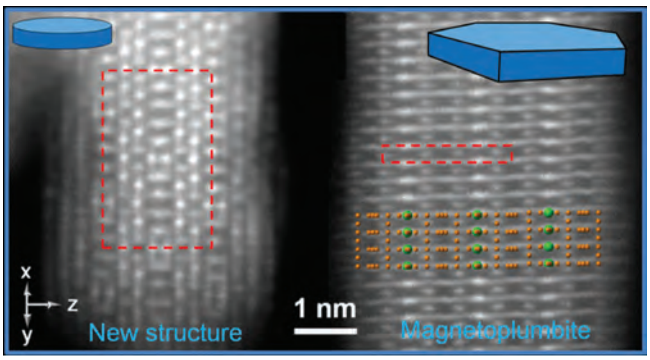

Figure 1: Atomic-resolution HAADF STEM images Sr-hexaferrite nanoplatelets. Left: initial nanoplatelet with new structure, right: nanoplatelet after exaggerated growth with magnetoplumbite structure.

different hexaferrite analogues on the hydrothermal synthesis of the nanoplatelets was systematically studied for different combinations of the there mentioned A-ions and different substituents.

A new metastable polymorph was also found during a systematic analysis of the hydrothermal synthesis of bismuth titanate ($Bi_4Ti_3O_{12}$). The bismuth titanate exhibits an Aurivillius structure that is formed from $(Bi_2O_2)^{2+}$ layers alternating with perovskite $(Bi_2Ti_3O_{10})^{2-}$ layers along the pseudo-tetragonal c-axis. Because of the layered structure, the bismuth-titanate nanoparticles tend to grow predominantly in the a/b plane to form rectangular nanoplatelets with the large surfaces parallel to the (001) crystal planes. However, numerous other nanostructures, including 1-D nanocrystals, nanowires of the bismuth titanate, were also synthesized. We found that the nanowires always appear in the initial stages of the bismuth titanate synthesis. Depending on the experimental conditions (e.g., the concentration of NaOH) they can transform to nanoplatelets or remain in the product. ARM analysis showed that the nanowires do not exhibit the Aurivillius structure of the bismuth titanate. The nanowires exhibit a new crystalline structure and actually represent a new polymorph of the bismuth titanate. With heating above 500 °C, the new structure of nanowire topotactically transforms to the equilibrium Aurivillius structure (Figure 2). Direct TEM imaging of a domain structure suggests that the nanowires are ferroelectric.

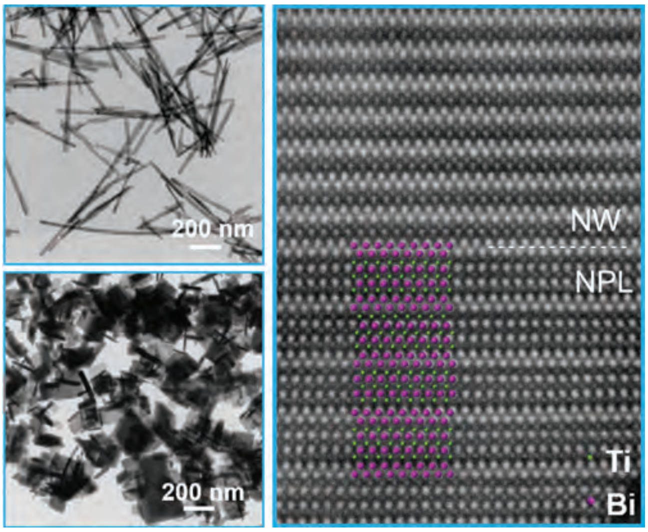

Figure 2: TEM images of bismuth-titanate nanowires (upper left) and nanoplatelets (bottom left). Right-hand-side image is atomic-resolution HAADF STEM of topotactic transformation from the new structure of nanowire (NW) to the Aurivillius structure characteristic for nanoplatelets (NPL).

For applications of the nanoparticles, as well as for their assembly into composite materials, the engineering of their surface properties is of key importance. The surface properties are engineered either by coating with an inorganic shell and/or by bonding different functionalization molecules onto the nanoparticles' surfaces.

In 2020 we completed the investigation on the deposition of a robust silica shell that contains large, radially aligned pores (Figure 3). A dynamic soft-templating strategy was developed to controllably synthesize hierarchical, dual-mesoporous silica shells on various core nanoparticles, in terms of nanoparticle dimensions (i.e., from 3 nm to micrometre), shape (i.e., spherical, chain-like, and disc-like), and magnetic properties (i.e., permanently magnetic and superparamagnetic). The developed interfacial co-assembly method 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 deposition method was applied for the syntheses of various magnetically guidable core-shell nanostructures. The versatility of the method was demonstrated by transferring the coating procedure from individual superparamagnetic iron-oxide nanoparticles to their clusters (Figure 3), nanochains (i.e., magnetically assembled chain-like agglomerates of nanoparticles clusters), and permanently magnetic hexaferrite nanoplatelets. This method can serve as a general approach to the fabrication of well-designed mesoporous silica coatings on a wide variety of core nanoparticles. The results were published in *ACS Applied Materials & Interfaces* (IF= 8.758).

Development of magnetic nanostructures, nanoclusters and nanochains with a highly porous silica shell for targeted drug delivery.

Apart from the silica coating, the functionalization molecules are grafted onto nanoparticle surfaces to control their surface properties. The layer of molecules has to be bonded by forming stable covalent bonds, not to be desorbed or exchanged with other ligands from the medium. Since irreversible covalent bonding is not possible between 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, sulfonates, phosphonates). Among those, the phosphonates are known to form the strongest coordinative bonds, especially with trivalent metals like Fe^{3+} and lanthanides. In our study we compared four different phosphonic acids for coating the surfaces of barium-hexaferrite nanoplatelets. The difference between them was in their functionality (mono-, di- and tetra-phosphonic acid) and polarity (from highly polar and completely soluble in water to nonpolar and insoluble in water). Few-nanometre-thick amorphous coatings formed under various synthesis conditions (ligand concentration, temperature, pH, time) from all four phosphonic acids. Highly porous coatings with specific surface areas of 600–700 m^2/g (comparable to metal-organic frameworks) were made of mono- and di-phosphonic acids with limited solubility in water. In contrast to this, both the polar and nonpolar mono-phosphonic acids formed dense bilayers on the surfaces of nanoplatelets. The formation of porous coatings was explained by a partial dissolution of the core nanoplatelets and the subsequent precipitation of a stable phosphonate framework. The new porous hybrid materials composed of an anisotropic magnetic core hybridized with a porous framework having many active sites (e.g.., -OH, P=O, P–O, =NH^+) were efficient in the purification of water from heavy metals. The study was made in cooperation with the Department for Complex Matter (Dr. Alenka Mertelj), Department for Nanostructured Materials (Dr. Andraž Kocjan), Department of Surface Engineering and Optoelectronics (Dr. Janez Kovač), Department of Physical and Organic Chemistry (Dr. Anton Kokalj), and University of Nova Gorica (Prof. Iztok Arčon, Prof. Matjaž Valant).

We continued the research related to the ferromagnetic suspensions of barium hexaferrite nanoplatelets (in cooperation with the Department of Complex Matter). We focused on our understanding of 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 showed that for making stable alcoholic ferromagnetic ferrofluids, the nanoplatelets need to be stabilized electrostatically with a dynamic double layer of the surfactant molecules. The condition for their stability is the possibility for a dynamic rearrangement of the surfactant layer(s) between the nanoplatelets' surfaces and the solvent. Consequently, nonpolar ferrofluids colloidally stabilized with steric repulsion were stable only for limited concentrations of the nanoplatelets, i.e., below the critical concentration for ferromagnetic coupling. A theoretical study related to these aspects was accomplished with the additional involvement of the University of Vienna, Austria, and Ural Federal University from Ekaterinbourg, Russia.

Actuation of magnetic nanoclusters with an AC magnetic field was applied to selectively heat the surface of a catalyst.

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 plane of the nanoplatelets, 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" (leader Dr Jelena Papan). The study was focused on the possibility to apply Pickering emulsions for the synthesis of such complex nanomaterials. The first barium hexaferrite – gold Janus nanoplatelets – were obtained after the optimization of the emulsification and hybridization processes. Two other projects started this year. A national project with the University of Ljubljana, Faculty of Chemistry and Chemical Technology 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 plane of the nanoplatelets. The second project is FET-OPEN MAGNELIQ project between our institute, University of Maribor, CNR Trieste, the Czech Academy of Sciences and an SME Prensilia from Pisa, in which we aim to develop a magneto-electric liquid based on magneto-electric Janus nanoplatelets.

We continued the research on clusters of superparamagnetic iron-oxide nanoparticles, i.e., nanoclusters. The nanoclusters are developed for applications that require a manipulation with an applied magnetic field. Their magnetic guidance enables a broad spectrum of applications, such as magnetic drug delivery, magnetic separation of poisonous heavy metals from water and even phospho-peptide enrichment from cancer cell lysates for further analyses. Here, we have demonstrated the use of magnetic nanoparticles in phosphoproteomics, where magnetically isolated phospho-peptides were analysed using NanoHPLC-MS/MS with selectivity as high as 90%. This interdisciplinary collaborative work was performed with researchers from different institutions in Italy and Portugal (Sapienza University of Roma, University of Trieste, University of Salento, Lecce, and University of Aveiro). The results were published in *Nano Research* (IF=8.18).

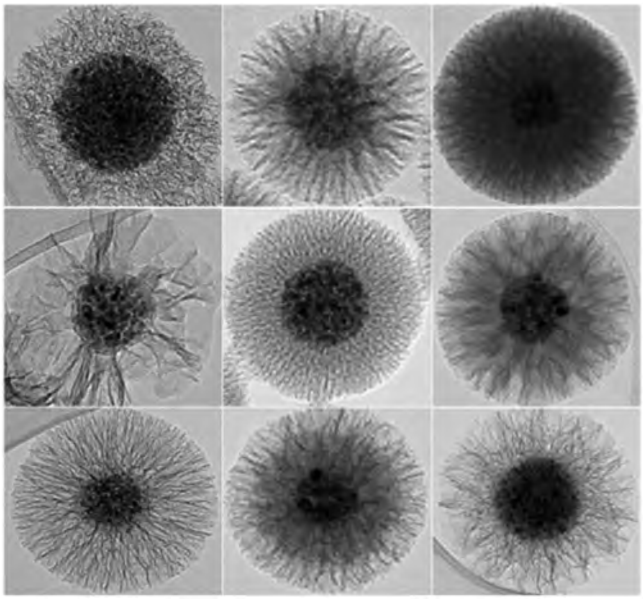

Figure 3: TEM images of superparamagnetic nanoparticle clusters coated with silica shells of diverse morphologies.

In cooperation with researchers from the Faculty of Pharmacy, University of Ljubljana (Prof Petra Kocbek) we continued studies on the development of magnetic drug-delivery systems. The nanoclusters were coated with silica having large and radially aligned pores (Figure 3). The pores in the silica enable loading of an active pharmaceutical substance, while the magnetic particle core provides magnetic guidance of the loaded drug-delivery system to the targeted tissues. The research on this topic is in progress.

In 2020 we completed two investigations on the magneto-rheology of biocompatible chain-forming ferrofluids with magnetic nanoclusters in collaboration with the researchers from University of Latvia, Riga, Latvia (Prof Dmitry Zablotsky and Prof Mikhail M. Maiorov). We studied the magnetorheological properties and structural transitions in novel aqueous colloidal suspensions of magnetic nanoclusters developed for biomedical applications. The region of intermediate magnetic coupling strengths between those observed in ferrofluids and in magnetorheological suspensions was systematically studied for the first time. Hybrid numerical simulations with hydrodynamic interactions provide full structural information. Analysis in terms of dimensionless parameters showed generalized behaviour, which is applicable to a broad class of magnetic suspensions.

We also continued the research on the application of the magnetic-heating of carbon and alumina-coated magnetic nanoclusters in the synthesis of catalysts and in catalysis. Both types of magnetic nanoclusters were prepared by thermal transformation of precursor materials. The precursors were synthesized by i.) hydrothermal carbonization of carbohydrate (for carbon-coated nanoclusters) or ii.) hydrolysis of AlN in the colloidal suspension of superparamagnetic iron-oxide nanoparticles (alumina-coated).

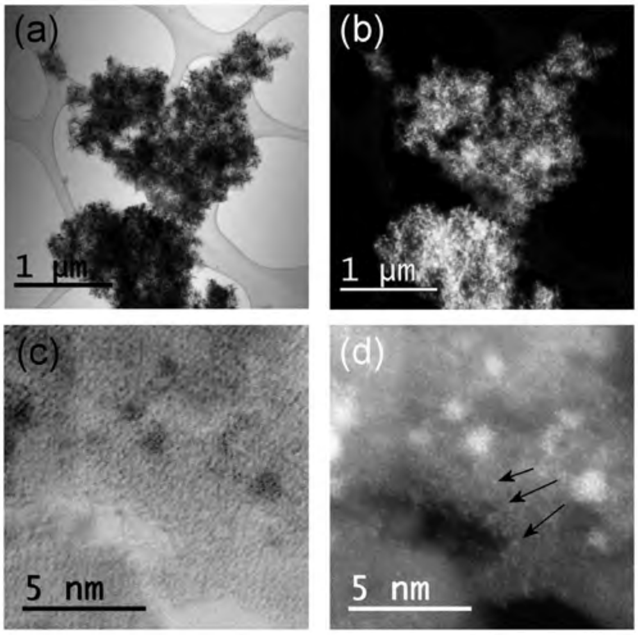

Figure 4: BF ((a) and (c)) and HAADF ((b) and (d)) STEM images of the RuNi/Al_2O_3 nanocatalyst. Ni atom clusters are marked with arrows.

As a proof of concept of the application of magnetic heating for the synthesis of nanomaterials, we synthesized bimetallic Ru and Ni bearing nanocatalysts using magnetic nanoparticles actuated with an alternating magnetic field (AMF) as a heat source for the reduction of Ru^{3+} and Ni^{2+}. The alumina-coated magnetic nanoclusters were impregnated with an aqueous solution of Ru^{3+} and Ni^{2+}, followed by drying under a reduced pressure. The impregnated nanoclusters were exposed to the AMF under the static atmosphere of H_2. The locally delivered heat led to the homogeneous deposition of Ru nanoparticles, approx. 2 nm in size, and Ni atom clusters exclusively on the surfaces of alumina-coated magnetic nanoclusters (Figure 4). Compared to the reduction with conventional heating, the time for nanocatalyst synthesis, i.e., the time needed to quantitatively reduce the Ru^{3+} and Ni^{2+}, was shortened from approximately 5 h to 10 min and the magnetically mediated heating-up and cooling-down periods were shortened, since the reaction medium remains at a significantly lower temperature than the nanocluster surfaces. We conducted preliminary catalytic tests that already showed promising results in collaboration with the Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry (Dr Blaž Likozar and Dr Miha Grilc).

In collaboration with the same research group from the National Institute of Chemistry we also studied AC-field-mediated catalysis using the 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 hydrogenation of levulinic acid. A relatively small amplitude of the field was sufficient for the hydrogenation to occur. Within 2 hours the conversion of levulinic acid reached almost 100 % and the selectivity for gamma-valerolactone was as high as 90 %. Microkinetic modelling was used to further study the process. The initial reaction rate under AC-field heating was significantly higher compared to the conventional heating. The estimated surface temperature of the catalyst was found to be in the range between 200 °C to 250 °C, while the bulk of the liquid medium reached only 120 °C. Such analysis rationalizes the 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.

Frustrated Lewis pairs are compounds where a Lewis acid and base cannot form a classic adduct because of steric hindrance. There are well known molecular examples and a few solid-state ones. Compounds are interesting because the energy of frustration can activate small molecules such as H_2, CO and CO_2, which are typically activated by precious, or on rare occasions, by transition metals. In collaboration with the University of Bern (Prof Ulrich Ashauer), Department of Nanostructured Materials (Dr Andraž Kocjan), Department of Inorganic Chemistry and Technology (Dr Gašper Tavčar and Dr Tomaž Skapin) and with the Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry (Dr Blaž Likozar and Dr Miha Grilc) we are investigating the influence of the surface acidity of aluminium oxide/fluoride and structure of the adsorbed Lewis base on their potential for formation of surface frustrated Lewis pairs and their hydrogenation activity. Theoretical calculations of the electric field between an adsorbed triphenylphosphine and Al^{3+} cation in fluoride showed that the field is relatively small due to a charge transfer between the molecule and the surface (the system loses some of its FLP character). The result suggests that H_2 dissociation is not spontaneous but facilitated. The reason for the charge transfer is most likely a too small ligand cone angle of the triphenylphosphine (< 180 °), meaning that the molecule is not sufficiently sterically hindered to form the frustrated Lewis pair on the surface of the aluminium fluoride. Currently, we are exploring (experimentally and theoretically) more sterically hindered molecules, such as tri-tert-butylphosphine.

We also continued with the research of fluorescent optical materials. Fluorescent nanoparticles with upconversion emission can be applied in various optical elements and are also proposed as alternative bio-markers in imaging diagnostic techniques for medicine. After our previous discovery of the significant dissolution of fluoride-based upconverting 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 upconverting nanoparticles. We showed that the coating-synthesis conditions are very important for making dense phosphonic coatings. All the coatings diminished the dissolution of the UCNPs by more than 50% when moderate heating is applied during the coating process. This is the result of the more efficient bonding of phosphonic acids with the surface rare-earth ions through the enhanced condensation reaction. Moreover, the dense coatings also showed an improvement of the cell viability when compared to the bare UCNPs. Another direction was to determine the effectiveness of polymeric coatings made from an amphiphilic poly(maleic anhydride-alt-1-octadecene) (PMAO) itself or additionally crosslinked with bis(hexamethylene)tri-amine (BHMT). We showed that the PMAO itself provided for better protection than any of the studied phosphonate coatings and that a subsequent crosslinking with BHMT did not provide for a substantial improvement. This means that the hydrophobic layer of the PMAO provided for an effective barrier that prevented the diffusion of water molecules and solute species to/from the UCNPs surfaces into the aqueous medium. The dissolution studies were made in cooperation with the Department of Inorganic Chemistry and Technology (Dr Maja Ponikvar-Svet) and 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 made at the Faculty of Medicine, University of Ljubljana (Dr Lovro Žiberna).

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 the dimensional changes at a phase transformation in the non-conducting phase, disconnections occur in the conductive phase that lead to the PTCR anomaly.

Some outstanding publications in the past year

1. Gyergyek, Sašo, Kocjan, Andraž, Grilc, Miha, Likozar, Blaž, Hočevar, Brigita, Makovec, Darko. Hierarchical Ru-bearing alumina/magnetic iron-oxide composite for the magnetically heated hydrogenation of furfural. *Green chemistry*, ISSN 1463-9262, [in press] 2020, 14 str.,
2. Goršak, Tanja, Drab, Mitja, Križaj, Dejan, Jeran, Marko, Lyubomirova Genova, Julia, Kralj, Slavko, Lisjak, Darja, Kralj-Iglič, Veronika, Iglič, Aleš, Makovec, Darko. Magneto-mechanical actuation of barium-hexaferrite nanoplatelets for the disruption of phospholipid membranes. *Journal of colloid and interface science*, ISSN 0021-9797, 1 Nov. 2020, vol. 579, str. 508-519,
3. Tadić, Marin, Milošević, Irena, Kralj, Slavko, Hanžel, Darko, Barudžija, Tanja, Motte, Laurence, Makovec, Darko. Surface-induced reversal of a phase transformation for the synthesis of- ε-Fe2O3 nanoparticles with high coercivity. Acta materialia, ISSN 1359-6454. [Print ed.], 2020, 27 str., doi: 10.1016/j.actamat.2020.01.058.

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 - 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. Anisotropic magnetic nanoparticles for the magneto-mechanical therapy of cancer
   Prof. Darko Makovec
2. Electrically tunable ferromagnetic liquids
   Prof. Darja Lisjak
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. Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF)
   Prof. Darko Makovec
   Ministry of Economic Development and Technology
7. Equipment use contract
   Asst. Prof. Sašo Gyergyek
   Inovine d. o. o.

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Original Article

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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:

Asst. Prof. Matjaž Spreitzer

Novel functional oxides

In the scope of the M-era.Net project "SunToChem", the engineering of perovskite photocatalysts was focused on the hydrothermal epitaxial growth of $SrTiO_3$ on $Bi_4Ti_3O_{12}$ nanoplatelets. An in-depth understanding of the mechanism for formation of $SrTiO_3/Bi_4Ti_3O_{12}$ is of broader importance for the design of two-dimensional (2D/2D) nanoheterostructures. Intimate contact on a larger surface in the 2D/2D heterojunction is expected to enhance the stability of composites and enables fast charge transfer, resulting in improved photocatalytic performance. Since a strong chemical bond between two semiconductors is formed during hydrothermal epitaxial growth, this is a promising approach for the preparation of new, efficient heterostructured photocatalysts. In the design of nanoheterostructures, electron band structure and crystal lattice matching of both semiconductors should be considered. The latter is crucial for successful epitaxial growth. $SrTiO_3$ and $Bi_4Ti_3O_{12}$ show a good structural match in the [001] $Bi_4Ti_3O_{12}$ || [100] $SrTiO_3$; {110} $Bi_4Ti_3O_{12}$ || (100} $SrTiO_3$ orientational relationship with the lattice spacings of {110} $Bi_4Ti_3O_{12}$ and {100}$SrTiO_3$ being 0.3842 nm and 0.3905 nm, respectively. Experimental conditions for the epitaxial growth were determined based on the thermodynamics for $SrTiO_3$ formation. Advanced methods of aberration-corrected electron microscopy allowed us to gain an in-depth insight into the microstructural characteristics of the initial $Bi_4Ti_3O_{12}$ precursor, $SrTiO_3/Bi_4Ti_3O_{12}$ interface, final $SrTiO_3$ platelets and thus describe the process of epitaxial growth in detail, down to the atomic scale. In this epitaxial growth, the $Bi_4Ti_3O_{12}$ platelets act as a source of $Ti(OH)_6^{2-}$ species and at the same time as a substrate for the epitaxial growth of $SrTiO_3$. The dissolution of the $Bi_4Ti_3O_{12}$ platelets proceeds faster from the lateral direction, whereas the epitaxial growth of $SrTiO_3$ occurs on both the bismuth-oxide-terminated basal surface planes of the $Bi_4Ti_3O_{12}$ platelets. In the progress of the TC reaction, the $Bi_4Ti_3O_{12}$ platelet is being replaced from the lateral ends toward the interior by the $SrTiO_3$, while the $Bi_4Ti_3O_{12}$ is preserved in the core of the heterostructural platelet. The mechanism of the epitaxial growth is presented in Figure 1.

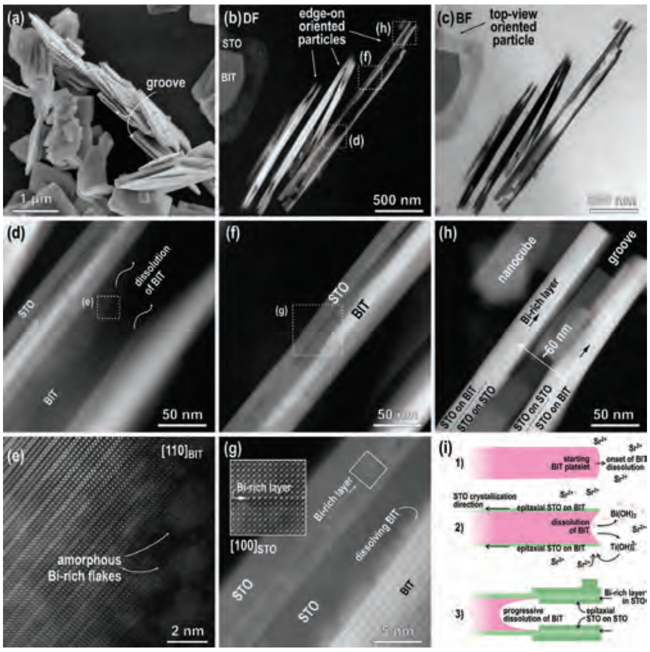

*Figure 1: (**a**) SEM and (**b-h**) STEM micrographs of $SrTiO_3/Bi_4Ti_3O_{12}$ heterostructural platelets (mainly edge-on-oriented platelets, which were thinned to electron transparency) as obtained after 1 h of a reaction at 200°C (6-M NaOH, Sr/Ti=12). (**b**) DF and (**c**) BF images showing (mainly) edge-on platelets along the whole side length, (**d**) DF of the central part of the platelet (showing $SrTiO_3$ layers and partially disintegrated $Bi_4Ti_3O_{12}$ inside the groove). (**e**) HR image of the area marked in (d) showing the disintegration of the $Bi_4Ti_3O_{12}$. (**f**) Another DF of the part between the central area and the edge of the platelet. (**g**) Magnified area from the image (f) presenting dissolution of the $Bi_4Ti_3O_{12}$ and the as-formed $SrTiO_3$ with the incorporated Bi-rich layer (HR image of this part is in the inset). (**h**) DF image of the edge of the platelet with two parallel $SrTiO_3$ platelets with incorporated Bi-rich layers. (**i**) Schematically shown processes of the TC reaction from $Bi_4Ti_3O_{12}$ to $SrTiO_3$ as reconstructed from STEM results, presented in b-h (ACS Applied Materials & interfaces, 13 (2021) 370-381).*

Since $SrTiO_3$ possesses more negative conduction band potential (E_{CB}) and Fermi level (E_F) than $Bi_4Ti_3O_{12}$, the electrons are transferred from $SrTiO_3$ to $Bi_4Ti_3O_{12}$ near the interface until Fermi-level equalization. This results in the formation of slightly positive and negative charge on the $SrTiO_3$ and $Bi_4Ti_3O_{12}$ sides, respectively. In the photocatalytic process, this internal electric field at the interface favour the migration of photogenerated electrons from the E_{CB} of $Bi_4Ti_3O_{12}$ to the valence band (E_{VB}) of $SrTiO_3$, where they recombine. Consequently, the photogenerated electrons in the E_{CB} of $SrTiO_3$ and holes in the E_{VB} of $Bi_4Ti_3O_{12}$ are available for the reduction of H^+ to H_2 and oxidation of methanol, respectively. This so-called direct Z-schemes mechanism explains the enhanced H_2 evolution on $SrTiO_3$/

$Bi_4Ti_3O_{12}$ nano-heterostructures. An in-depth understanding of the reaction mechanism for the formation of $SrTiO_3$/$Bi_4Ti_3O_{12}$ platelets expands the possibility of using the hydrothermal epitaxial growth approach for the design of other 2D/2D hetero-structural photocatalysts.

Without any support from noble-metal doping or co-catalysts, the $SrTiO_3$/$Bi_4Ti_3O_{12}$ platelets show a considerably higher photocatalytic H_2 evolution than individual materials and commercial $SrTiO_3$. The explanation for the improved photocatalytic performance of $SrTiO_3$/$Bi_4Ti_3O_{12}$ nanoheterostructural platelets was established based on the electronic band structures of $SrTiO_3$ and $Bi_4Ti_3O_{12}$.

A large emphasis of our research was on the integration of functional oxides with silicon using the pulsed-laser deposition technique. This year we focused on the mechanisms for the formation of a silicate layer at the junction between a $SrTiO_3$ thin film and a silicon substrate. The formation of such interlayers is not desirable because it prevents the transfer of electric charge across the STO-Si junction and therefore their use in certain applications. We found that by repeating the annealing to crystallize the STO layer, the thickness of the silicate interlayer is gradually increased to values of 1.2–1.9 nm. On the other hand, the expansion of the silicate layer does not significantly affect the quality of the STO layer itself. A crystallographic analysis using the XRD technique with a synchrotron light source has shown that ~3.7-nm-thick STO layers are highly crystalline, single-phase, and can be used for the epitaxy of thicker STO films, which was confirmed with additional experiments. XRD investigations also showed that thin layers of STO predominantly exhibit a cubic unit cell with a slightly larger unit cell (u.c.) volume compared to the bulk STO u.c. volume. The increase in the u.c. volume indicates the presence of oxygen vacancies in the STO films, which is a consequence of performing the STO deposition in an inert atmosphere. The results of this research will help us to further optimize the process for the growth of STO thin films on silicon.

A part of the research in the field of HfO_2 thin-film synthesis was carried out as part of the postdoctoral training of dr. Urška Trstenjak at the Peter Grünberg Institute (PGI-7), Forschungszentrum Jülich. HfO_2 is a material that exhibits interesting electrical properties, while being compatible with established processes in the electronics industry. The purpose of our work was to study the growth of HfO_2 thin films prepared by pulsed-laser deposition on amorphous substrates coated with graphene. Unlike the conventional preparation of epitaxial thin layers directly on crystalline substrates, in the synthesis on graphene the film binds to the substrate via van der Waals forces which enables dislocation-free strain relaxation. In the first phase of research, we focused on the prevention of graphene oxidation during the growth of the oxide film. We found that the use of bilayer graphene most effectively maintained the integrity of the graphene layers. The second-most important role was played by the gas atmosphere during deposition, where the growth of HfO_2 at a relatively high Ar pressure protected the graphene better than the deposition under UHV conditions, which is attributed to a decrease in the kinetic energy of the plasma particles, leading to reduced mechanical deformation of graphene. We found that graphene plays a key role in the successful crystallization of HfO_2 on SiO_2 substrates. We also found that HfO_2 on graphene grows in a thermodynamically stable monoclinic phase. By changing the deposition conditions, we were able to influence the crystallographic texture of the film.

The use of a high Ar pressure decreases the kinetic energy of the plasma particles and consequently reduces the mechanical deformation in the graphene layer.

We continued the study of growth and functional properties of the relaxor ferroelectric $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT) thin films. In particular, we were interested in studying the effect of the epitaxial strain in thin films with a thickness < 100nm. The principal aim was the growth of high-quality epitaxial relaxor ferroelectric PMN-PT thin films, which, in turn, enables the investigation of the role of biaxial misfit strain in driving changes to the domain structures and piezoelectric and ferroelectric response of the functional layer. PMN-33PT/SRO heterostructures were grown using pulsed-laser deposition on atomically smooth and singly-terminated oxide single-crystalline $SrTiO_3$ (STO) and $ReScO_3$ (*Re*= Dy, Tb, Gd, Sm, and Nd) (RSO) substrates (with a rocking curve value <0.05°). These substrates permit the application of a wide range of compressive strains on the PMN-33PT films from -2.90% (STO substrate) to -0.10% (NSO substrate). To avoid the pyrochlore phases and the deficiency in lead and magnesium (produce stoichiometric PMN-33PT thin films), 20 mol. % PbO and 10 mol.% MgO excess were used in the targets. We controlled the epitaxial growth mode at the unit-cell level of the deposited materials using *in-situ* high-pressure reflection high-energy electron diffraction (RHEED); first for the SRO on singly terminated STO and RSO substrates and then for the PMN-33PT layer on the SRO/STO and SRO/ RSO templates. RHEED and high-resolution X-ray diffraction (HR-XRD) analysis confirmed high-quality and epitaxial single-phase thin films with smooth 2D surfaces. Combining HR-XRD reciprocal space maps (RSMs) and HR-STEM investigations, fully strained PMN-33PT/SRO heterostructures free from defects were revealed on DSO, TSO, GSO, and SSO substrates with sharp interfaces confirming the 2D cube-on-cube growth mode of both SRO and PMN-33PT layers. In addition, from the RSMs patterns, an evolution from butterfly-shaped diffraction pattern for mildly strained PMN-33PT layers, which is evidence for the stabilization of relaxor domains, to disc-shaped diffraction patterns for high compressive strains with a highly distorted tetragonal structure, was revealed (Figure 2). The PFM amplitude and phase of the PMN-33PT thin films confirmed the relaxor-like response for a strain state below ~1.13%, while, for higher compressive strain (~1.9%), the irregularly shaped and poled ferroelectric domains were observed. Interestingly, the PFM phase hysteresis loops of the PMN-33PT heterostructures grown on the SSO substrates (strain state of ~ 0.8%) exhibited an enhanced coercive field, which is about two times larger than that of the thin films grown on GSO and NSO substrates. The obtained results demonstrated that the domain structures of the PMN-33PT heterostructures are sensitive to the applied compressive strain and this later could serve as an effective approach for tailoring and enhancing the functional properties in relaxor ferroelectrics.

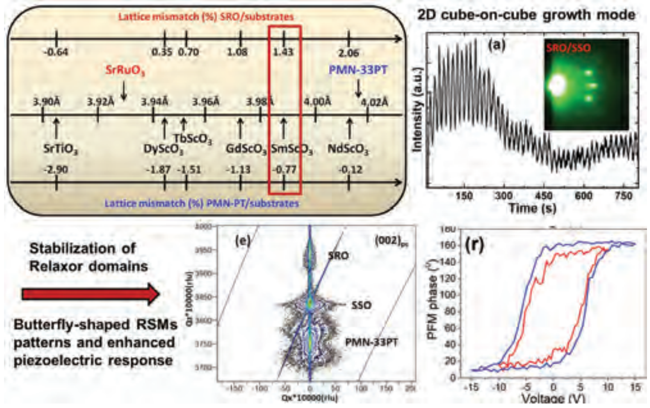

Figure 2: Strain engineering in epitaxial PMN-33PT films revealing a butterfly-shaped diffraction pattern for mildly strained films, evidencing the stabilization of relaxor nanodomains.

In collaboration with CRISMAT-CNRS Laboratory (Caen, France) we investigated thermoelectric materials inspired by the natural mineral colusite with complex crystal structure. The compound belongs to a new class of environmentally friendly copper-based sulphides composed of abundant, low-cost, industrial-grade raw materials. Mechanical alloying in combination with spark plasma sintering was used for the synthesis. The approach leads to the formation of various types of nano-to-microscale defects, from local Sn-site structural disorder to nano-inclusions and vanadium-rich core-shell microstructures (Figure 3a). We studied the recrystallization mechanism from the initial elements to the final colusite at different sintering temperatures. The analyses showed that metallic vanadium particles react with the surrounding copper sulphides to the transient V-rich sulvanite, Cu_3VS_4 (Figure 3b). Further diffusion processes lead to the formation of a V-rich and Sn-deficient colusite phase with a chemical composition around $Cu_{26}V_4Sn_4S_{32}$ with a V:Sn ratio of 1:1, and finally to the V-Sn colusite phase, $Cu_{26}V_2Sn_6S_{32}$ (Figure 3c). Multiscale defects in the final colusite grains have a strong impact over phonon scattering, making it possible to reach ultra-low lattice thermal conductivity. Simultaneously, the electrical transport properties are impacted through variations in charge-carrier concentration and effective mass, leading to a synergistic improvement of both the electrical and thermal properties. The results of this study were performed in the frame of the national research project J1-9177 and are published in Acta Materialia.

Structural inhomogeneities affect the phonon scattering and increase the charge-carrier density, leading to a synergistic improvement of the thermal as well as electrical properties.

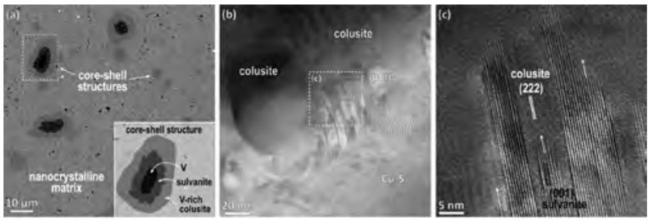

Figure 3: (a) V-rich core-shell structures in the sample after SPS at 600°C. (b) Transition between Cu-sulphide to colusite over transient sulvanite phase. (c) Oriented recrystallization of sulvanite to colusite.

In the scope of an investigation of phase relations in ternary oxide systems where new compounds and solid solutions form and exhibit interesting electric properties, we determined high-temperature phase equilibria in the La_2O_3–TiO_2-Nb_2O_5 system and presented it as a ternary phase diagram. In the system we identified numerous solid solutions based on already known compounds as well as one new solid solution. Extensions of the solid solutions were determined by systematic sample preparation and additional precise analysis. We also identified one new ternary compound and determined its chemical composition. The two-phase ceramics based on one subsystem exhibit very interesting microwave dielectric properties, which can be tailored by changing the relative content of the end components. Thus, the temperature-stable dielectric properties can be achieved at a certain composition.

Our research in the field of functional oxides that exhibit dielectric properties also included "upside-down" ceramic composites based on Li_2MoO_4–$SrTiO_3$ (LMO-ST), prepared by room-temperature fabrication (RTF) as a sustainable alternative to the time- and energy-consuming high-temperature sintering of ceramics (Figure 4). In the scope of our study, various physical parameters that might affect the overall processing and their final dielectric performance, were investigated. LMO-ST composites are based on a high ratio of filler ST, coupled with the corresponding LMO binder. During the room-temperature pressing and subsequent drying at 110°C, the binder proceeds to crystallize on the surface of the filler particles. Consequently, the filler particles become physically bound and the overall porosity decreases (ρ_{rel} = 84%). The experimental results in the low-frequency measurement area (1MHz) exhibit a relative permittivity

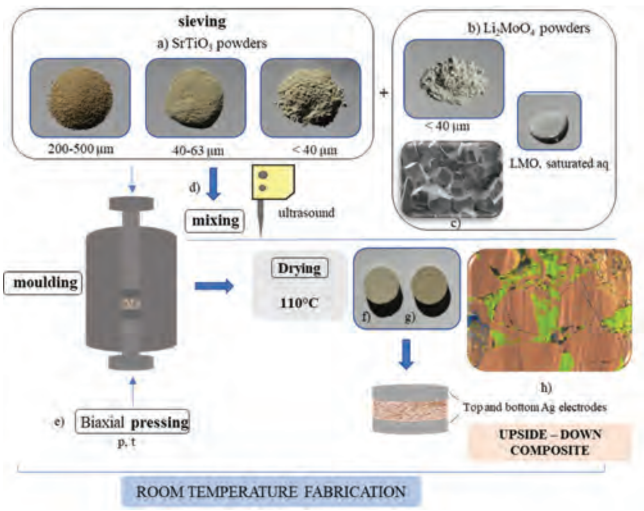

Figure 4: Experimental preparation protocol of upside- down LMO-ST composites is presented on the processing scheme.

(ε_r) of 65–78 corresponding with dielectric losses (tan δ) of 0.002–0.05. The properties can attract considerable attention for the utilization of LMO-ST composites in the industry of electroceramics.

Zinc (Zn) is an essential micronutrient in human health and is the reason for the massive annual production of zinc glutonate-based food additives and medicines. Unfortunately, once expired, waste zinc gluconates are generally disposed of 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. To reduce environmental pollution and the waste of zinc resources, we investigated the recycling of expired waste zinc gluconate as a source for preparation of photocatalytic ZnO nanostructures. In a typical synthesis, zinc gluconate water solution was placed in a Teflon container, sealed in an autoclave and hydrothermally reacted at 180 °C/12 h. The resulting black suspension was washed, centrifuged and dried. Black powder was fired at 500°C. The XRD analysis has shown that the obtained powder consisted of the ZnO wurzite compound with a 45-nm particle size. However, an SEM investigation has shown ZnO micron spheres that consisted of nanoparticles intertwined with a hollow structure. We have shown that such a structure enables good photocatalytic activity by testing the degradation of the organic methyl blue dye under the UV light, which has shown that 50 % of the dye degrades in 90 min.

Antibacterial and piezoelectric biocompatible materials

With the aim to create novel tools applicable in regenerative medicine and tissue engineering, we are working on designing novel biomaterials with the focus in two areas: designing organic piezoelectrics and developing innovative antimicrobials.

Within the project Mechano-chromic, voltage-sensitive electrostimulators: innovative piezoelectric biomaterials for electro-stimulated cellular growth, in collaboration with partners from ETH, Switzerland, we are developing biocompatible and biodegradable organic piezoelectric films designed to accelerate cellular proliferation. For this purpose, we optimized two processing approaches: drawing and template wetting. Drawing enables thick poly-l-lactide (PLLA) piezoelectric films with a layered structure (Figure 5a). Upon mechanical deformation using ultrasound, films dropped in cell growth media can generate a voltage signal. We observed that biodegration of these films starts as surface erosion due to their hydrophilic surface, which preserves their mechanical and piezoelectric properties for a longer period of time under simulated physiological conditions. The template-wetting method provides nanotextured PLLA films containing aligned nanotubes with approximately 100-nm diameters (Figure 5b). By observing single nanotubes using XRD and polarized Raman, we confirmed that crystallization and molecular orientation are the key properties needed to obtain piezoelectricity. Both types of films, layered and nanostructured, are confirmed to have antibacterial characteristics as a consequence of piezo-stimulation. In the case of nanotubes, piezoelectricity is combined with a nanotexture, which additionally contributes to their antimicrobial performance. In contrast to their effect on bacterial cells and providing antibacterial properties, piezoelectric PLLA films, both layered and nanotextured, do not trigger any haemolysis and damage in animal-sourced red blood cells (RBCs). Staining RBC membrane do not reveal any mechanical damages after piezostimulation and membrane non-permeable FM 646 dye remained on their outer leaflet (Figure 5d).

The optimal functionalization that prevented particle aggregation and further growth in aqueous media was obtained by replacing oleic acid with dopamine ligands.

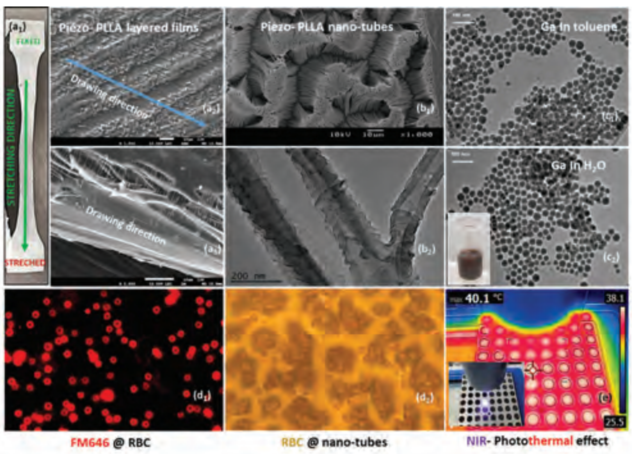

Figure 5: Piezo-PLLA films in the form of layered structure ($a_{1\text{-}3}$) and nanotubes ($b_{1\text{-}2}$). Gallium nanoparticles: from hydrophobic (c_1 in toluene) to hydrophilic (c_2 stable suspension in water). Red blood cells (RBCs) labelled with FM646 (surface impermeable) (d_1) and on top of nanotubes (d_2). NIR laser irradiating nanoparticles and their heating (e).

We also continued our research on developing novel antimicrobial nanomaterials. Within the project Environmentally friendly antimicrobial material for textile with improved properties, together with the Centre for Technology Transfer (CTT) we collaborate with the Hungarian company Innowear-tex, as anti-microbial textile producer, and Portugal industrial textile research institute (CITEVE). Together we are developing and testing a textile prototype containing antimicrobial components based on functionalized gold, initially developed and patented in our lab. In addition, we worked on the preparation of stable aqueous colloidal solutions of monodisperse gallium nanoparticles with different sizes and surface ligands to investigate their antibacterial properties in detail. Starting from a thermal decomposition synthesis that yields monodisperse oleic-acid-capped Ga nanoparticles, we changed the surface properties from hydrophobic to hydrophilic using different ligand-exchange processes. The optimal results were obtained by replacing oleic acid with dopamine ligands (with morphology and water-stability illustrated in Figure 5c). We have explored the influence of near-infrared (NIR) laser irradiation on local heating of doped cobalt ferrite and their composites with functionalized gold nanoparticles to enhance their antimicrobial activity with the photothermal effect. The heating capacity of the composites obtained upon laser-irradiation is illustrated in Figure 5e. We consider the newly optimized Ga NPs as the most optimal for further antimicrobial studies, particularly as a new platform for photothermal antimicrobial activity.

Materials for heat-insulation applications

Insulation materials have a strong impact on the energy efficiency of buildings, which are one of the main energy-consumers, representing 40 % of all consumed energy in the EU. The use of waste raw materials and less energy-intensive processes are important trends in scientific research, aiming to reduce the industrial impact on the environment.

In accordance with these trends, we investigated the use of waste container glass in foamed-glass production. However, due to the poor glass stability of container glass, i.e., its tendency towards crystallization, it is difficult to obtain a product with a good quality. We investigated crystallization in the container glass by DSC and XRD analyses and observed a complex crystallization with the separation of several crystalline phases. The glass stability improves if the glass is re-melted and becomes similar to the stability of a model soda-lime-silica glass prepared from technical grade chemicals. However, it remains unsuitable for foam-glass production. Therefore, we tested various additives in order to inhibit the crystallization. Finally, we succeeded to inhibit the crystallization process with the selection of the proper fluxing agents (B_2O_3 or borax) in a combination with crystallization inhibitor Al_2O_3. XRD analysis revealed that with the addition of fluxing agents the crystalline content decreased to below 15% and these results are also evidenced by DSC analyses. Measurements of the thermal conductivity on the sintered-glass samples confirmed the important decrease of thermal conductivity by inhibition of the crystallization. Based on the obtained knowledge on the crystallization process, we tested foaming mixtures with the fluxing additives and observed the best results for the addition of B_2O_3. The closed porosity decreased, as expected, due to the smaller crystalline content. However, it was not possible to decrease the density to suitably low values. Therefore, we continued with the development of the foaming recipe by moderately decreasing the content of B_2O_3 and the introduction of phosphates, with the aim to decrease the viscosity and surface tension. The results we obtained are promising and the future focus will be on the preparation of larger foam samples for characterization of the thermal and mechanical properties.

Optimization of the new foaming recipe, containing a combination of fluxing additives and crystallization inhibitor, led us to promising results.

The use of waste materials in combination with water glass can further decrease the environmental impact of foamed-glass production, while maintaining high-quality product characterized by low thermal conductivity. Water glass is a well-known and commonly used additive for foamed-glass production. However, the related foaming mechanisms are scarcely investigated and while a commonly accepted mechanism theory exists, it is not supported by experimental evidence (Figure 6). With the use of waste panel cathode-ray-tube (CRT) glass, which exhibits good glass stability, we focused on revealing the mechanisms of glass foaming with water glass. We analysed the behaviour of the foaming mixture of CRT and water glass during heating via heating stage microscopy (HSM) and thermogravimetry coupled with mass spectroscopy (TG/MS). The atmosphere inside the closed pores of the foamed glass were investigated by gas chromatography (GC/MS), which revealed that, surprisingly, CO_2 is the main component. The results showcase the sensitivity of the foaming mixture on the atmospheric CO_2 which reacts with hydrated layer of glass and forms carbonates. Newly formed carbonates decompose at elevated temperatures, producing CO_2, which is the driving force behind the expansion. Additionally, foaming process can be controlled by controlling the degree to which the reaction between hydrated layer of glass and CO_2 can proceed. We found that this can be achieved by drying the foaming mixture, i.e. freeing it of “low-temperature” water, which inhibits the reaction. Future research will be focused on the exploitation of newly revealed mechanisms to produce sustainable foamed glass.

Figure 6: Higher addition of water glass allows the same expansions to be achieved at lower temperatures, which has a favourable effect on the energy complexity of production.

Projects

As part of the **M-ERA-NET project: SunToChem**, researchers from the Jožef Stefan Institute (JSI), the Institute of Solid State Physics, the University of Latvia (ISSP-UL) and the Department of Chemical Engineering of the National University of Taiwan (CHe-NTU) are pooling the latest knowledge in the field of particle morphology design (JSI), theoretical calculations (FP) and photocatalytic measurements (ChE-NTU) to prepare efficient perovskite photocatalysts for the formation of H_2 by water cleavage. The main purpose of the project is to precisely control particle characteristics such as exposed surface types, finishes, crystal defects (oxygen gaps), mesocrystallinity, hetero-structuredness, and ferroelectricity to increase photocatalytic efficiency based on better charge-carrier separation and light absorption. Funded by: M-ERA.NET European transnational agency. Coordinator: dr. Marjeta Maček Kržmanc

Applied project **Mineral wool composites with improved insulation properties** is focused on the development of a new, innovative preparation procedure for mineral wool composites with decreased thermal conductivity. Theoretical calculations on the thermal conductivity of the composites were experimentally validated, confirming the great potential of the new composites. Testing of mechanical properties of the composites revealed that modifications to the surface properties is necessary to obtain suitable stability of the composite. Surface properties of the composite's components properties were modified by thermal and chemical routes. The results showed that any excessive amount of water used in the processing is detrimental for mechanical as well as insulation properties. Thereafter, investigation focused on the development of a dry composite processing route, which gave the best results in terms of mechanical and insulation properties. The dry processing route also has the highest industrial feasibility. Funding agency: Slovenian Research Agency. Coordinator: Jakob König.

Project **SIOX** aims to exploit the rich functionalities of oxides and their heterostructures, which show great promise within the emerging field of oxide electronics. For their implementation, the epitaxial integration of oxides with silicon platforms using industrially appropriate technology is urgently needed, and its development represents the main goal of SIOX. Funding agency: M-ERA.NET European Transnational Agency. Coordinator and principal investigator: Asst. Prof. Matjaž Spreitzer.

Awards and appointments

1. Heli Jantunen: Yushan Scholar Award, Yushan, Taiwan, Ministry of Education (MOE), ROC Taiwan, Ultra-low temperature co-firing ceramics.
2. Matjaž Spreitzer, Srečo Škapin: Silver award of the CCIS for the innovation TCG Autoskimm, Maribor, Chamber of Commerce and Industry of Slovenia, Development of automatic slag skimming process to reduce aluminum losses and ensure reproducible melt quality.
3. Matjaž Spreitzer, Srečo Škapin: Silver award of the CCIS for the innovation New super-light and super hard engineering materials, Maribor, Chamber of Commerce and Industry of Slovenia, Development of a laboratory-verified synthetic pathway for the production of lightweight, super-solid advanced materials based on Al-Mg-B-Ti.
4. Matjaž Spreitzer: Success Story - ENPIEZO, Austria, M-era.Net Network, Innovative Surfaces, Coatings and Interfaces: Enabling technology for high-quality piezoMEMS.
5. Danilo Suvorov, Srečo Škapin, Marija Vukomanović: Special prize for innovations for economy, Ljubljana, Center for technology transfer and innovation JSI, Contact-based, leaching-free antimicrobial textile Silver-free, wearable germ protection.
6. Marija Vukomanović: Success Story within KETGate project, Interreg Central Europe, Ljubljana, Center for technology transfer and innovation JSI, Development of products based on nanofibers with potential antimicrobial effect for various applications.

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", 11. 6. 2020 & 9. 12. 2020 (virtual).
2. Kick-off meeting of international project "Mechano-chromic, voltage-sensitive electrostimulators: innovative piezoelectric biomaterials for electro-stimulated cellular growth", 15. 9. 2020 (virtual).
3. Kick-off meeting of international project KET4Clean Production: "Environmentally friendly antimicrobial material for textile with improved properties", 21. 9. 2020 (virtual).
4. Workshop on international project M.ERA-NET "SIOX: Engineering of silicon-oxide interface using the pulsed-laser deposition technique", 20.7. 2020 (virtual).

INTERNATIONAL PROJECTS

1. Investigation of NdDyCoCuFe Rare Earth Alloys Alloys and Related Compounds
   Asst. Prof. Matjaž Spreitzer
   Urban Mining Company
2. Investigation of NdDyCoCuFe Rare Earth Alloys Alloys and Related Compounds
   Asst. Prof. Matjaž Spreitzer
   Urban Mining Company
3. COST CA 17140; Cancer Nanomedicine - From the Bench to the Bedside (NANO2CL)
   Asst. Prof. Marija Vukomanović
   Cost Association Aisbl
4. Stoichiometry Engineering of Epitaxial PMN-PT Thin Films
   Asst. Prof. Matjaž Spreitzer
   Slovenian Research Agency

RESEARCH PROGRAMME

1. Contemporary Inorganic Materials and Nanotechnologies
   Asst. 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. Piezoelectric Biomaterials for Electro-stimulated Regeneration
   Asst. Prof. Marija Vukomanović
4. Nanoscale investigations of diffusion controlled topotaxial phase transformations in rutile-corundum host systems
   Asst. Prof. Nina Daneu
5. Engineering of oxides on silicon for future electronics
   Asst. Prof. Matjaž Spreitzer
6. Mineral inclusions in garnet from macroscopic to atomic scale: Opening the petrogenetic archive
   Asst. Prof. Nina Daneu
7. Strain and domain structure engineering in epitaxial relaxor ferroelectric thin films
   Asst. Prof. Matjaž Spreitzer
8. Mechano-chromic, voltage-sensitive electrostimulators: innovative piezoelectric biomaterials for electro-stimulated cellular growth
   Asst. Prof. Marija Vukomanović
9. Engineering of relaxor ferroelectric thin films for piezoelectric and energy storage applications
   Asst. Prof. Matjaž Spreitzer
10. Mineral wool composite with improved insulation properties
    Dr. Jakob König
11. Central European SME Gateway zo Key-enabling Technology Infrastructures - Sparking new Transnational KET Innovation Ecosystem
    Asst. Prof. Matjaž Spreitzer
    Bay Zoltan Alkalmazott Kutatasi Kozhasznu
12. Innovative ECO plasma seed treatment (for sowing and for human and animal diet/nutrition
    Asst. Prof. Marija Vukomanović
    Ministry of Education, Science and Sport
13. Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF)
    Asst. Prof. Matjaž Spreitzer
    Ministry of Economic Development and Technology
14. Control of crystallization in glass materials for thermal insulation
    Dr. Sonja Smiljanić
    Ministry of Education, Science and Sport
15. HarvEnPiez: Innovative nano-materials and architectures for integratedpiezoelectric energy harvesting applications
    Dr. Marjeta Maček Kržmanc
    Ministry of Education, Science and Sport
16. SIOX: Engineering of silicon-oxide interface using the pulsed-laser deposition technique
    Asst. Prof. Matjaž Spreitzer
    Ministry of Education, Science and Sport
17. SunToChem: Engineering of perovskite photocatalysts for sunlight-driven hydrogen evolution from water splitting
    Dr. Marjeta Maček Kržmanc
    Ministry of Education, Science and Sport
18. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
    Asst. Prof. Matjaž Spreitzer
    Slovenian Research Agency
19. XRD Analysis
    Asst. Prof. Matjaž Spreitzer
20. Stay of Nina Kuzmić iin Oulu, Finland - Low Temperature Densification of Strontium Titanate Ceramics, May - June 2020
    Nina Kuzmić
    Jecs Trust
21. KET4CLEAN-INNOWEAR-TEX; Costs of Work of K9 on the Case KET4CLEAN PRODUCTION-INNOWEAR-TEX
    Asst. Prof. Matjaž Spreitzer
    Innowear-tex Kft.

VISITORS FROM ABROAD

1. Dr. Manal Benyoussef, Laboratoire de Physique de la Matière Condensée (LPMC), Amiens, France, 27. 1. to 13. 3. 2020 and 1. 6. to 30. 9. 2020.
2. Dr. Taisia Alifirova, Department of Lithospheric Research, University of Vienna, Austria, 19. 7. to 24. 7. 2020.

Visiting Researchers

1. Dr. Saswati Santra, Indian Institute of Science, Bangalore, India, 15. 2. to 31.8. 2020.
2. Dr. Jamal Belhadi, Laboratoire de Physique de la Matière Condensée (LPMC), Amiens, France, 1. 3. 2019 to 29. 2. 2020.
3. Dr. Sonja Smiljanić, University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia, 1. 6. 2019 to 31.3. 2022.

STAFF

Researchers

1. Asst. Prof. Nina Daneu
2. Heli Maarit Jantunen, B. Sc.
3. *Zoran Jovanović, left 05.01.20*
4. Dr. Jakob König
5. Dr. Gertjan Koster
6. Dr. Špela Kunej
7. Dr. Marjeta Maček Kržmanc
8. **Asst. Prof. Matjaž Spreitzer, Head**
9. Prof. Srečo Davor Škapin
10. Dr. Marija Vukomanović

Postdoctoral associates

11. Jamal Belhadi, B. Sc.
12. *Dr. Sonja Jovanović, left 05.01.20*
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PUBLISHED CONFERENCE CONTRIBUTION

1. Katja Traven, Mark Češnovar, Srečo D. Škapin, Vilma Ducman, "Evaluation of fly ash-based alkali activated foams at room and elevated temperatures", In: *2nd International Conference on Technologies & Business Models for Circular Economy*, Proceedings, Maribor Faculty of Chemistry and Chemical Engineering, 2020, 23-34.
2. Tina Radošević, Anja Černoša, Manca Kovač Viršek, Martina Kocijan, Damjan Vengust, Cene Gostinčar, Aleš Mihelič, Nina Gunde-Cimerman, Sašo Šturm, Matejka Podlogar, "Razgradnja tekstilnih mikroplastičnih vlaken s fotokatalizo in glivami", In: *Vodni dnevi 2020, 17.-18. september 2020, Rimske Toplice, Kongresni center Rimske terme*, zbornik referatov, Slovensko društvo za zaščito voda, 2020, 203-213.

THESES AND MENTORING

1. Janvit Teržan, *Propene partial oxidation with molecular oxygen over alkali modified CuO_x/SiO_2 catalysts:* doctoral dissertation, Ljubljana, 2020 (mentor Matjaž Spreitzer; co-mentor Petar Djinović).

DEPARTMENT OF BIOCHEMISTRY, MOLECULAR AND STRUCTURAL BIOLOGY B-1

The research activities of the members of the department are largely focused on studies of the physiological role of proteases and their endogenous protein inhibitors in normal and pathological conditions, the mechanism of their action and regulation, as well as their properties and structure. As molecular mechanisms of protease action are only partially understood, since only a limited number of physiological substrates of a few proteases has been identified, a lot of work remains to be done.

Head:
Prof. Boris Turk

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, cancer, cardiovascular, neurologic and neurodegenerative disorders. Thus, proteases represent an extremely important group of targets for therapeutic intervention.

In cancer studies we have shown that L-leucyl-leucine methyl ester (LLOMe), a lysosomotropic detergent, influences cell death and this depends on the levels of cathepsin C. We have shown that the deletion of the endogenous cathepsin inhibitor stefin B results in sensitizing primary murine breast-cancer cells to cell death without affecting the release of cathepsins, whereas the simultaneous ablation of cathepsins B and L largely protects mouse embryonic fibroblasts against cell death. However, due to the extreme sensitivity of monocytes to LLOMe, it appears that the drug may not be suitable for anticancer therapy due to a risk of systemic toxicity (Kavčič et al., 2020).

As we know from animal models cancer studies, the specific inhibitory affinity of proteases can be utilized for targeted drug delivery. We confirmed before the selective targeting of cathepsins by stefin A-conjugated liposomes *in vitro* and *in vivo* and demonstrated the potential of this approach for cancer diagnostics and treatment. In the last year we summarized our studies in a review paper (Vizovišek et al., 2020), where we gave expert opinion on the potential of cysteine cathepsins as therapeutic targets in inflammation-associated diseases. We described the direct targeting of cathepsins for treatment purposes and their indirect use in diagnostics. The targeting of cysteine cathepsins has not translated into the clinic; this failure is attributed to off- and on-target side effects and/or the lack of companion biomarkers. This field now embraces developments in diagnostic imaging, the activation of prodrugs and antibody-drug conjugates for targeted drug delivery. The future lies in improved molecular tools and therapeutic concepts that will find a wide spectrum of uses in diagnostic and therapeutic applications.

In the continuation of our protease-specificity studies, we performed the proteomic characterization of cysteine proteases gingipains from the bacteria P. gingivalis, causing periodontitis (Hočevar et al., 2020). HRgpA and RgpB gingipains have Arg-specificity, while Kgp gingipain is Lys-specific. Together they can cleave an array of proteins and importantly contribute to the development of periodontitis. We focused on gingipain-exerted proteolysis at the cell surface of human gingival epithelial cells [telomerase immortalized gingival keratinocytes (TIGK)] in order to better understand the molecular mechanisms behind tissue destruction in this disease of the gums. Using mass spectrometry, we investigated the whole sheddome/degradome of TIGK cell surface proteins by *P. gingivalis* strains differing in gingipain expression and by purified gingipains, and performed the first global proteomic analysis of gingipain proteolysis at the membrane. Most of the identified gingipain substrates were molecules involved in adhesion, suggesting that gingipains can cause tissue damage through the cleavage of cell contacts, resulting in cell detachment and rounding, and consequently leading to anoikis.

In a review paper (Biasizzo and Kopitar Jerala, 2020) the interplay between NLRP3 Inflammasome and autophagy is discussed. Namely, the NLRP3 inflammasome is a cytosolic multi-protein complex that induces inflammation and pyroptotic cell death in response to both pathogen and endogenous activators, leading to the formation of the inflammasome complex, which results in the activation of caspase-1, followed by the cleavage and release of pro-inflammatory cytokines. The excessive activation of NLRP3 inflammasome can contribute to the development of inflammatory diseases and cancer. Autophagy is a vital intracellular process for recycling and the removal of damaged proteins and organelles, as well as the destruction of intracellular pathogens. The autophagy dysfunction can lead to diseases with hyperinflammation and excessive activation of NLRP3 inflammasome and thus acts as a major regulator of inflammasomes. Autophagic removal of NLRP3 inflammasome activators, or NLRP3 inflammasome components, and cytokines can reduce inflammasome activation.

In collaboration with Joel Selkrig and Athanasios Typas, EMBL Heidelberg, Germany, we reported on the trafficking of lysosomal cysteine cathepsins to the extracellular space and to the nucleus upon infection with *Salmonella enterica Typhimurium*. Typas' lab used a proteomics approach to selectively quantify newly synthesized host proteins during infection. Nuclear cathepsin activity was required for pyroptotic cell death via the non-canonical inflammasome activation. Nuclear targeting of a cathepsin inhibitor, stefin B or pharmacological cathepsin inhibition suppressed *S. enterica* Typhimurium-induced cell death. Moreover, cathepsin inhibition reduced the expression of gasdermin D, a key protein in pyroptotic cell death (Sekrig et al., 2020).

Apart from cysteine cathepsins, several aspects of their endogenous inhibitors, stefins and cystatins are studied by our group. For example, stefins are being used as model proteins to study protein folding and aggregation. We have determined the effect of polyphenols and vitamin C and some other anti-oxidants on protein aggregation (Jahić et al., 2020). Polyphenols, such as curcumin, are mostly inhibiting protein aggregation, which maybe explains their neuroprotective role as protein misfolding and aggregation are involved in neurodegenerative diseases. We are using the amyloidogenic protein stefin B as a prototype of amyloidogenic proteins and explore its pore formation, for which we have started collaboration with the group of biophysics (Štrancar's lab) and hope to see protein oligomers in interaction with cellular membranes.

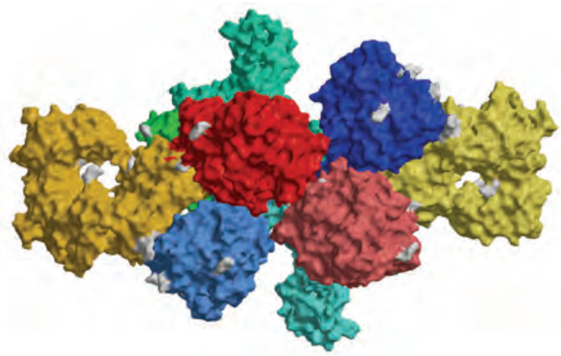

Figure 1: Thyroglobulin is a dimer, formed by two polypeptide chains. The surface representations shows the structure colored according to the structure divided in regions: N-terminal domain (blue), core (cyan), flap (green), arm (yellow), C-terminal domain (red). To differentiate the polypeptide chains, one is shown with dimmed colors.

The most important work that resulted in the determination of the 3D structure of human thyroglobulin, the protein precursor of thyroid hormones, which are essential for growth, development and the control of metabolism in vertebrates, was done in collaboration with the group of Jan Loewe from MRC Cambridge (UK) (Coscia et al., 2020). The structure of full-length human thyroglobulin at a resolution of approximately 3.5 Å was determined by cryo-electron microscopy. We identified all of the hormonogenic tyrosine pairs in the structure, and verified them using site-directed mutagenesis and in-vitro hormone-production assays using human thyroglobulin expressed in HEK293T cells. Our analysis revealed that the proximity, flexibility and solvent exposure of the tyrosines are the key characteristics of hormonogenic sites. We transferred the reaction sites from thyroglobulin to an engineered tyrosine donor-acceptor pair in the unrelated bacterial maltose-binding protein, which yielded hormone production with an efficiency comparable to that of thyroglobulin. Our study thus provides a framework to further understand the production and regulation of thyroid hormones.

In addition, the group for structural biology determined several structures of bacterial enzymes that can contribute to the development of novel antibacterial drugs. In pursuit of novel drug targets for the human pathogen S. aureus, we thus studied peptidoglycan N-acetylglucosaminidases, whose structures are composed of two domains forming a V-shaped active site cleft. Combined insights from crystal structures supported by site-directed mutagenesis, modelling, and molecular dynamics enabled us to elucidate the substrate-binding mechanism of SagB and AtlA-gl. This mechanism requires domain sliding from the open form observed in their crystal structures, leading to polysaccharide substrate binding in the closed form, which can enzymatically process the bound substrate. We suggest that these two hydrolases must exhibit unusual extents of flexibility to cleave the rigid structure of a bacterial cell wall (Pintar et al., 2020). The second target was SecA protein, a major component of the general bacterial secretory system. It is an ATPase that couples nucleotide hydrolysis to protein translocation. In some Gram-positive pathogens, a second paralogue, SecA2, exports a different set of substrates, usually virulence factors. To identify SecA2 features different from SecA(1)s, we determined the crystal structure of SecA2 from Clostridioides difficile, an important nosocomial pathogen, in apo and ATP-γ-S-bound form (Lindič et al., 2020).

In addition, we collaborated with research groups from Slovenia and numerous other countries (Germany, Hungary, Croatia, Poland, United Kingdom, Netherlands, Japan and USA).

Some outstanding publications in the past year

1. Kavčič, N, Butinar, M, Sobotič, B, Hafner Česen, M, Petelin, A, Bojič, L, Zavašnik-Bergant, T, Bratovš, A, Reinheckel, T, Turk, B. Intracellular cathepsin C levels determine sensitivity of cells to leucyl-leucine methyl ester-triggered apoptosis. (2020) *FEBS journal*, 287(23):5148-5166.
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3. Coscia, Francesca, Taler-Verčič, Ajda, Chang, Veronica T., Sinn, Ludwig, O'reilly, Francis J., Izoré, Thierry, Renko, Miha, Berger, Imre, Rappsilber, Juri, Turk, Dušan, Löwe, Jan. The structure of human thyroglobulin. (2020) Nature, 578, 627-630.

Patents granted

1. Stephen James Moore, Margaret Thy Luu Nguyen, Daniel Robert Hostetter, Olga Vasiljeva, Jeanne Grace Flandez, Substrates of matrix metalloproteinase and other cleavable moieties and methods of use thereof, AU2014324884 (B2), Australian Patent Office, 26. 03. 2020.
2. James William West, Li Mei, Stephen James Moore, Margaret Thy Luu Nguyen, Daniel Robert Hostetter, Olga Vasiljeva, Jason Sagert, Jonathan Terrett, Anti-PDL1 antibodies, activatable anti-PDL1 antibodies, and methods of use thereof, US10669339 (B2), US Patent Office, 02. 06. 2020.

INTERNATIONAL PROJECTS

1. Supply of DPPI Enzyme and the Non-exclusive License Rights
   Prof. Dušan Turk
   Prozymex A/s
2. COST CA 15203; Mitochondrial Mapping: Evolution-Age-Gender-Lifestyle-Environment
   Prof. Nataša Kopitar – Jerala
   Cost Office
3. COST CA15124; NEUBIAS - A New Network of European Bioimage Analysts to Advance Life Science Imaging
   Asst. Prof. Tina Zavašnik Bergant
   Cost Office
4. COST CA15214; An Integrative Action for Multidisciplinary Studies on Cellular Structural Networks
   Prof. Nataša Kopitar – Jerala
   Cost Office
5. The Role of Cystatins in Neuroinflamamtion
   Prof. Nataša Kopitar – Jerala
   Slovenian Research Agency

RESEARCH PROGRAMMES

1. Structural biology
   Prof. Dušan Turk
2. Proteolysis and its regulation
   Prof. Boris Turk

R & D GRANTS AND CONTRACTS

1. Cathepsin X inhibitors impair the resistence of tumor cells to antiprotease therapy
   Prof. Boris Turk
2. Molecular genetic biomarkers and mechanisms of unresponsiveness to biological therapyanti-TNF in patients with chronic immune diseases
   Prof. Boris Turk
3. Structural insight into the mechanism of Clostridium difficle surface formation
   Prof. Dušan Turk
4. Inhibition of Staphylococcus aureus cell wall remodeling
   Prof. Dušan Turk
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. Innovative ECO plasma seed treatment (for sowing and for human and animal diet/nutrition
    Prof. Boris Turk
    Ministry of Education, Science and Sport
11. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
    Prof. Boris Turk
    Slovenian Research Agency
12. Lyposomal Proteases in Semaphorin Signaling and Cell Polarity
    Prof. Boris Turk
    Icgeb - International Centre For Genetic

NEW CONTRACT

1. Collaboration on quantification of cellular proteins by LC-MS/MS based proteomic analysis
   Prof. Marko Fonović
   Lek d. d.

VISITORS FROM ABROAD

1. Nora Diéguez Martínez, Barcelona University (UAB), Barcelona, Spain, 13 January to 14 March 2020
2. Gian Pietro Pietri, University of Rijeka, Croatia, 3-10 October 2020

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15. Dr. Nataša Lindič
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18. Dr. Jure Pražnikar*
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38. Maja Orehek, B. Sc.
39. Dejan Pelko
40. Polonca Pirš

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* part-time JSI member

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Theses and Mentoring

1. Andreja Bratovš, *Targeting the tumor microenvironment with nanoparticles for treatment and diagnostics:* doctoral dissertation, Ljubljana, 2020 (mentor Olga Vasiljeva; co-mentor Boris Turk).
2. Katarina Hočevar, *Role of extracellular cysteine proteases in the processing of membrane proteins:* doctoral dissertation, Ljubljana, 2020 (mentor Boris Turk).

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. 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 disease (AD).

In this year we continued 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 the 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. To this end, we prepared recombinant AtxA and rat GIIA, and their enzymatically inactive D49S mutants to synthesize different molecular tools, nanogold- and Alexa-derivatives. Using these tools, we studied the cellular trafficking of $sPLA_2s$ by electron- and fluorescent confocal microscopy, and confirmed their internalization in PC12 cells. By heterologous competition experiment, we demonstrated that rat GIIA only weakly competed with ^{125}I labelled Atx (^{125}I-Atx)-binding to CCOX subunit II. Consistently, upon labelling of porcine mitochondrial membranes with ^{125}I-GIIA, the CCOX subunit II was not labelled, but another protein of 20 kDa was. These two results suggest that the GIIA binding site on the CCOX is different from that of the Atx, but both binding sites overlap to some extent. According to the apparent molecular mass of the GIIA-binding protein, this protein might represent subunit IV of the CCOX that is in contact with subunit II in the CCOX complex. We demonstrated that GIIA inhibits the activity of the CCOX both *in vitro* and *ex vivo* in sections of rat brain tissue. This led us to hypothesize that the regulation of ATP production is another physiological function of GIIA in mitochondria (Figure 1). In pathological conditions, for example in AD, the expression of GIIA is significantly increased and the damage inflicted on neuronal mitochondria is very similar to that observed in the Atx-poisoned nerve endings. We have been trying to establish the link between the interaction of GIIA with CCOX and the degeneration of mitochondria, which is potentially very important for the early diagnosis of AD and its subsequent treatment.

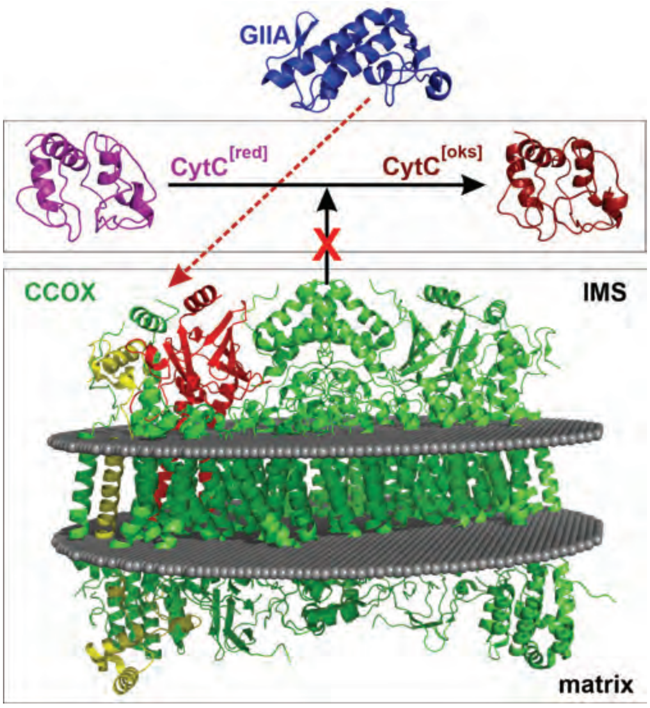

Figure 1: We proposed the regulation of ATP production as another physiological function of GIIA in mitochondria. Snake venom or mammalian group IIA phospholipase A_2 (GIIA) enters the intermembrane space (IMS) of mitochondria and binds to cytochrome c oxidase (CCOX), the former to its subunit II (red), while the latter most likely to its subunit IV (yellow). By binding to CCOX, either GIIA inhibits enzymatic activity of CCOX – the oxidation of cytochrome c (CytC) – downregulating in this way the production of cellular energy (ATP) by the respiratory chain.

We prepared a set of recombinant human $sPLA_2$ molecules, GV and GX, as well as their enzymatically inactive mutants, GV(H48Q) and GX(H48Q). These molecules, together with the rat and snake venom $sPLA_2s$ that have been synthesized before, will be used in electrophysiological studies to probe their effects on the nicotinic acetylcholine receptor (nAChR). Unfortunately, due to the Covid-19 pandemics, these experiments could not be performed as planned, in the scope of the bilateral project between Slovenia and the Russian Federation (BI-RU/19-20-029). Instead, they will be accomplished with a new partner, the Laboratory of Toxicology and Pharmacology from the Catholic University of Leuven in Belgium. In collaboration with the group from the University of Padova, our recombinant AtxA has been used to study the mechanism of regeneration of AtxA-degenerated motor axon terminals.

We wrote the first draft of a review paper that focuses on the antiviral action of both endogenous mammalian and exogenous (animal venom) $sPLA_2s$.

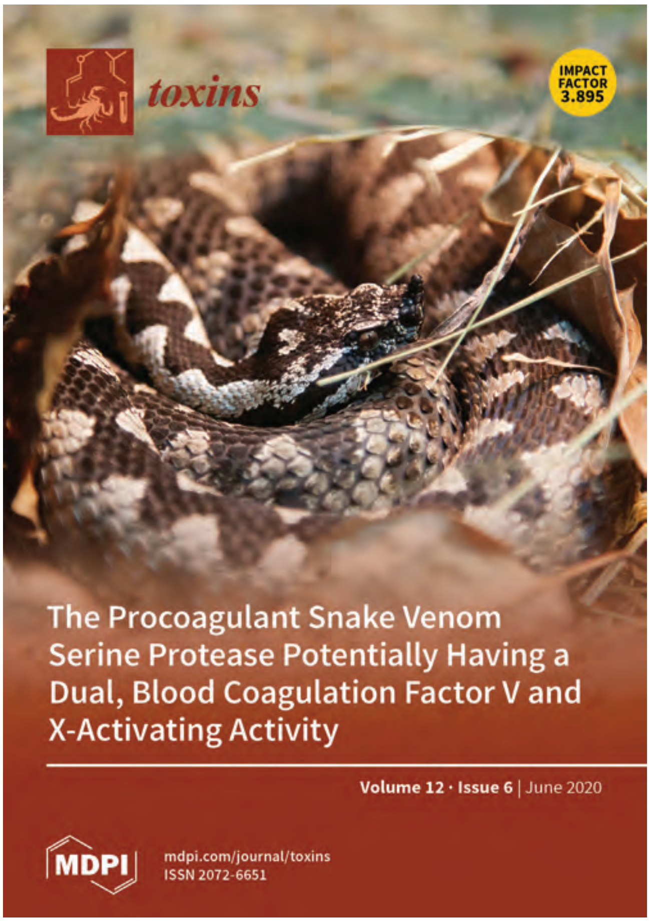

Figure 2: Cover page of the June issue of Toxins highlighted our paper inside. Venoms of the Viperidae snakes are rich in proteins that strongly affect the haemostatic system. Our study describes the isolation, purification and characterisation of an interesting procoagulant serine protease from the venom of the most venomous viper in Europe, the nose-horned viper (Vipera a. ammodytes). The blood-coagulation-promoting effect of VaaSP-VX, as the glycoprotein was named, is most likely based on a simultaneous activation of the blood-coagulation factors V and X, precursors of the prothrombinase complex. A unique proteolytic specificity along with the resistance to serpin inhibition endow VaaSP-VX with a promising medical potential, for example, for treating patients with haemophilia.

In 2020 we continued an intensive study of the snake-venom proteins that affect the blood-coagulation process – haemostasis. We finally succeeded in obtaining a 3-year research project J1-2475 from the Slovenian Research Agency (SRA) to boost our studies of a unique serine protease-like anticoagulant protein from the nose-horned viper venom, VaaSPH-1, with the ambition to create novel, safe anticoagulant drugs.

The results on VaaSP-VX, a serine protease with procoagulant, blood coagulation factor VIIa-like activity from the venom of the nose-horned viper (*Vipera a. ammodytes*, *Vaa*), were published in *Toxins* (Z. Latinović et al., *Toxins*, 12 (2020), 358). The very interesting discovery of the first procoagulant snake venom serine protease with dual, blood-coagulation factor V- and X-activating activity was highlighted on the cover page (Figure 2).

We performed an extensive characterization of the first member of a novel P-IIIe subclass of snake-venom metalloproteinases, lacking the entire catalytic (metalloproteinase) domain, VaaMPIII-3. Our partners from the Institute of Molecular Genetics and Genetic Engineering in Belgrade, Serbia, provided a vector to produce it in bacterial cells. Besides the biochemical point of view, we analysed this unique venom protein also from the pathophysiological point of view by describing its effects on blood coagulation (K. Požek et al., in preparation). In addition, within the scope of our international project on the whole *Vaa* genome sequencing, we obtained a contig of about 23 kb, presumably harbouring the *VaaMPIII-3* gene. Its nucleotide sequence and overall structure, composed of 10 exons and 9 introns, are importantly different from those of the *Eoc89-like* gene encoding a similar but catalytically active MPIII metalloproteinase from the viperid snake *Echis ocellatus*. It has also been confirmed that the lack of the metalloproteinase domain in VaaMPIII-3 is not a result of alternative mRNA splicing, but rather due to the corresponding genomic sequence, with a deletion of both the catalytic and subsequent part of the disintegrin domain-coding region, being present already at the gene level.

Zorica Latinović, our doctoral student in this area of research, was awarded the Krka Special Commendation Prize for her PhD thesis entitled "Components of the nose-horned viper venom that affect cardiovascular system".

In collaboration with colleagues from the University of Zagreb (UZ), we studied toxic activities of the venom of a very rare Croatian karst viper (*Vipera ursinii macrops, Vum*) and comprehensively described its proteomic profile. This snake is not medically important; however, its ecology is very special and it is threatened with extinction. Our data opened the way to unravel a unique insecticidal activity of the venom, potentially leading to new pesticides. Comparing the pathological properties of the *Vum* venom with those of the *Vaa* venom, and the proteomes of both venoms, we indicated the existence of neurotoxins in viperid venoms structurally unrelated to $sPLA_2$s (M. Lang Balija et al., *Toxins*, 12 (2020), 187).

Together with researchers from the Veterinary Faculty of the University of Ljubljana (UL), we finalised a study of the first Kunitz-type proteins from viperid venoms that potentiate neuromuscular transmission, and published our results (S. Drofenik et al., *Toxicon*, 187 (2020), 262–270). In this work we characterized the Kunitz-type proteins in *Vaa* venom. These proteins, VaaChi, potently inhibit serine proteases, particularly chymotrypsin. Most interestingly, we found that they also facilitate neurotransmission in a manner like that of α-dendrotoxin. They also significantly increased the amplitude of the indirectly evoked simple muscle contraction of the mouse hemidiaphragm, and the amplitudes of the end-plate potentials (EPPs) and miniature end-plate potentials (MEPPs). VaaChi are thus Kunitz-type proteins with dual functionality, representing the first examples of Kunitz-type proteins from viperid venoms affecting neurotransmission. What the mechanism is behind the facilitation of neuromuscular transmission by VaaChi has not been established; however, blocking of K^+ channels, as in the case of α-dendrotoxin, does not seem to be the most probable option. For this work, the student Sabina Drofenik received the Student Prešeren Award at the University of Ljubljana.

In collaboration with colleagues from the Centre for Clinical Toxicology and Pharmacology, University Medical Centre Ljubljana (UMCL), we investigated an interesting clinical effect, a profound, transient and reversible thrombocytopenia of functional platelets in patients envenomed by the nose-horned viper venom. In thrombo-embolic diseases, such as myocardial infarction and ischemic stroke, platelets play a pivotal role. Currently used antiplatelet drugs have one common side effect – a decreased count of platelets with an inhibited function. Such a condition represents a high risk of life-threatening haemorrhage, especially in interventional cardiology and angiology employing antithrombotic approach. Our findings might pave the way to the development of a new group of antiplatelet agents that will minimise the risk of life-threatening bleeding in an antithrombotic approach to interventional cardiology and angiology, and increase the effectiveness of vessel dilatation and emboli aspiration. As we demonstrated, reversible thrombocytopenia in patients poisoned by the *Vaa* venom is caused by snake C-type lectin-like proteins (snaclecs). To deepen these studies, we succeeded in obtaining a 3-year research project J3-2534 from the ARRS in 2020.

Animal venoms are rich source of new substances and molecular tools to improve human and animal health.

In the scope of a network including experts from UMCL, the University Hospital and the University of Split, the UZ and our group, we analysed samples collected from patients, envenomed by the nose-horned viper venom and treated with different antivenoms. We submitted a paper for publication in *Clinical Toxicology* suggesting new directives for efficient immunotherapy of the nose-horned viper envenomation (T. Kurtović et al., submitted).

In 2020 we also joined the COST Action "European Venom Network" (CA19144 - EUVEN), an excellent opportunity for establishing new international research collaborations.

Lipid metabolism and signalling

Our work in this area is focused on the identification of metabolic and signalling pathways that control lipid acquisition, trafficking and utilization in cancer cells. The resilience of cancer cells to stress depends on the availability of extracellular lipids and on their capacity to synthesize, mobilise or recycle their own intracellular lipids. By studying the ways in which cancer cells use lipids, we aim to reduce their remarkable ability to adapt to the inhospitable tumour micro-environment and thus reduce tumour growth, metastasis and resistance to therapy.

In 2020 our experimental work was focused on the final studies on the involvement of lipid droplets in the production of lipid mediators, such as prostaglandins and leukotrienes that are known promoters of inflammation and tumourigenesis (Figure 3). We have found that lipid droplets transiently store and regulate the release of polyunsaturated fatty acids, which are required to produce inflammatory lipid mediators. This work is important because it reveals that targeting lipid metabolism in cancer could represent a novel strategy for reducing inflammation and inflammation-related tumorigenesis. The validity and relevance of the acquired preliminary results were confirmed by awarding a post-doctoral research grant to Eva Jarc Jovičić (Z3-2650) by ARRS in 2020.

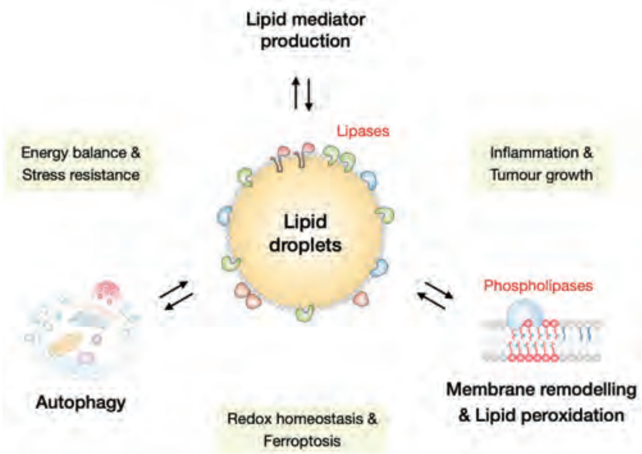

Figure 3: Lipid droplets are organelles that connect metabolic pathways with inflammation and the resistance of cancer cells to stress. Lipid droplets are in the core of our research work. These organelles are not only fat-storage repositories, but also active modulators of lipid peroxidation, autophagy and the production of inflammatory lipid mediators. By controlling these important aspects of cell biology, they are involved in the maintenance of the energy and redox balance as well as the regulation of inflammation in the tumour micro-environment that fosters tumour growth.

We have continued our work on the ARRS research project J7-1818 ("Targeting lipid droplets to reduce cancer cell resistance to stress"), where we are tackling the question of the cooperation between autophagy and lipid droplets in cancer cells. We opened a new, promising research field by focusing some of our efforts on investigating the role of lipid droplets in the protection of cancer cells from ferroptosis, a lipid peroxidation-induced form of cell death. Our networking efforts in this field have gained an important impetus by joining the COST Action – "Pan-European Network in Lipidomics and EpiLipidomics" (CA19105 - EpiLipidNET). We were also awarded a grant for a comprehensive proteomic work within the INSTRUCT-ERIC research network hub (PID13338 – "Identification of lipid droplet-associated ferroptotic modulators in cancer"). Our recent work in the field of lipid droplets has been accepted very well by the scientific community, as judged by the rapid increase in citations of our work and the invited lectures by Toni Petan at the 15th CFGBC Scientific Symposium and at the 1st COST EpiLipidNet meeting. Eva Jarc Jovičič also received the Krka Special Commendation Prize for her PhD thesis entitled "The role of lipid droplets in cancer cell stress resistance".

As part of a special volume of the journal *Reviews of Physiology, Biochemistry and Pharmacology* on "Organelles in Disease", we published an invited review paper entitled "Lipid droplets in cancer" (T. Petan, *Rev. Physiol. Biochem. Pharm.*, (2020), PMID 33074407). In this comprehensive review, we discuss emerging evidence showing that lipid droplets are important parts of cancer metabolic reprogramming. We explore how these fat-laden but highly dynamic organelles consolidate lipid uptake, synthesis, recycling, distribution and breakdown in order to match these entangled lipid fluxes with the requirements for cancer-cell survival, growth and metastasis. We focus on the mechanisms that govern lipid droplet function during metabolic stress and reveal their connections with autophagy and ferroptotic cell death. Finally, we discuss how dysregulated lipid droplet turnover can be detrimental to cancer cells, thereby providing exciting therapeutic opportunities in the future. In 2020 our second invited review paper on lipid droplets appeared. This one in the special issue of *Biochimie* (E. Jarc & T. Petan, *Biochimie*, 169 (2020), 69–87), in which we discussed the principal ways of regulating the availability of fatty acids by these organelles for the production of lipid mediators and the activation of inflammatory signalling pathways.

Targeting lipid-droplet metabolism in cancer cells is a promising strategy to reduce tumour growth.

We contributed to a study led by our colleagues from the National Institute of Chemistry. In 2020 we published the paper in a prestigious journal (V.T. Ha et al., *Proc. Natl. Acad. Sci. USA*, 117 (2020), 25679–25689), in which we revealed a new mechanism of the activation of inflammatory pathways by stress-induced extracellular vesicles containing oxidized lysophospholipids. The latter are produced by the synergistic activities of 15-lipoxygenase and GIIA $sPLA_2$, which are upregulated during inflammation and can be therapeutically targeted in inflammatory diseases such as rheumatoid arthritis. Our expertise in $sPLA_2$ enzymology, cell biology and the production of recombinant proteins was a key contribution to this important work.

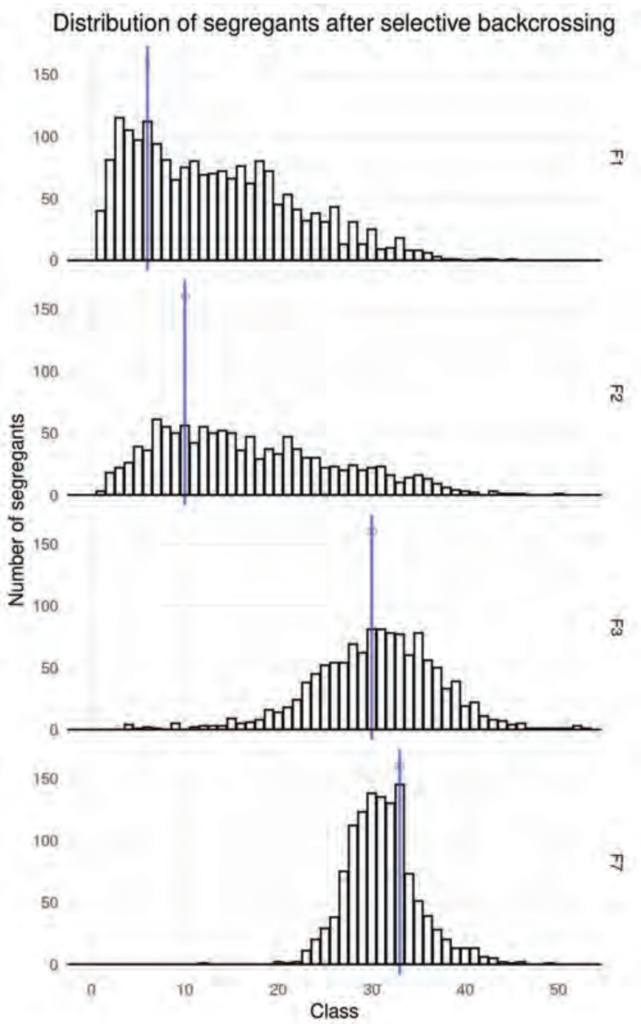

Figure 4: Identification of halotolerance quantitative trait loci (QTL). Two yeast strains with different halotolerance were crossed and sporulated. One thousand individual segregants after each round of backcrossing were assessed for their ability to grow in the presence of NaCl in a high-throughput manner. In each generation, the winner was chosen and back-crossed with its parental strain. The distribution shows the gradual improvement in mean halotolerance of each generation. Based on persistent genomic markers through generations, quantitative trait loci were predicted.

High-throughput genetics and functional genomics in yeast *Saccharomyces cerevisiae*

Most of the biotechnologically important traits of micro-organisms are polygenic, which is one of the reasons for the focus of our research on polygenic traits in yeast *S. cerevisiae*. We performed a comprehensive study demonstrating how backcrossing and high-throughput phenotyping can be used to identify quantitative trait loci (QTLs) for sodium chloride tolerance (Figure 4). We expanded our own method for the iterative crossing of genetically diverse yeast strains to identify causative genetic elements for an extremely high level of acidotolerance. We continued to develop our CRISPR-Cas multiplex method, ensuring that we now possess all the necessary technologies to start developing multi-trait industrial yeast strains.

We finished our work on a project on environmental condition- and variant-dependent binary physical interactions between selected yeast proteins, which was part of a large consortium's project on the proteome-scale maps of binary protein interactions. We have been using the same basic method – yeast two-hybrid assay – to develop an approach that can discriminate between pathogenic and non-pathogenic variants of the human protein MLH1, thus offering an accurate and relatively quick method to clinical geneticists with Lynch syndrome patients.

Genetics and genomics of yeasts for the development of biotechnology.

Evolutionary genomics

The diversity and evolution of RNA viruses has been well studied in arthropods and especially in insects. However, the diversity of RNA viruses in the basal hexapods has not been analysed yet. To understand their diversity better, evolutionary histories and genome organizations, we searched for RNA viruses in the transcriptome and genome databases of basal hexapods. We discovered ~40 novel RNA viruses, some of which are also present as endogenous viral elements derived from RNA viruses. We demonstrated that basal hexapods host 14 RNA viral clades that have been recently identified in invertebrates. The following RNA viral clades are associated with basal hexapods: Reo, Partiti-Picobirna, Toti-Chryso, Mono-Chu, Bunya-Arena, Orthomyxo, Qinvirus, Picorna-Calici, Hepe-Virga, Narna-Levi, Tombus-Noda, Luteo-Sobemo, Permutotetra and Flavi. We have found representatives of the 9 RNA viral clades that are present as endogenous genomic copies in the genomes of Machilis (Monocondylia) and Catajapyx (Diplura). Our study provided a first insight into the diversity of RNA viruses in basal hexapods and demonstrated that the basal hexapods possess quite a high diversity of RNA viral clades (S. Ott Rutar and D. Kordiš, *Peer J.*, 8 (2020), e8336).

Evolutionary, genomic and structure-function analysis of viruses, receptors and satellite DNA.

Honeybees play a crucial role in global food production as pollinators of numerous crops. Several stressors cause declines in populations of managed and wild bee species, such as habitat degradation, pesticide exposure and pathogens. Viruses act as the key stressors and can infect a wide range of bee species. Most honeybee-infecting viruses are RNA viruses of the Picornavirales order. Although some ssDNA viruses are common in insects, such as densoviruses, they have not yet been found in honeybees. Densoviruses were, however, discovered in bumblebees and ants. In this paper we demonstrated that densoviruses are indeed present in the transcriptome of the eastern honeybee (*Apis cerana*) from southern China (S. Ott Rutar and D. Kordiš, *Acta Agric. Slov.,* 116 (2020), 383–393). Based on non-structural and structural transcripts, we inferred the genome structure of the *Apis* densovirus. Phylogenetic analysis has shown that this novel Apis densovirus belongs to the *Scindoambidensovirus* genus in the Densovirinae sub-family. Apis densovirus possesses ambisense genome organisation and encodes three non-structural proteins and a split VP (capsid) protein. The availability of the complete Apis densovirus genome will enable the analysis of its potential pathogenic impact on honeybees. Our findings will certainly foster the research of densoviruses in honeybees and bumblebees.

Satellite DNAs are major constituents of centromeric and pericentromeric regions in many eukaryotes and their role in centromere and kinetochore assembly and heterochromatin formation has been extensively investigated. However, the role of satellite repeats found dispersed in euchromatin, outside of centromere/pericentromere regions, remains largely unexplored. We analysed the dynamics of dispersion for human α-satellite repeats throughout euchromatin during the evolutionary history of primates and the mechanism of their proliferation (I. Feliciello et al., *Genome Biol. Evol.*, 12 (2020), 2125–2138). These results contribute to the understanding of evolutionary and functional significance of satellite DNA repeats spread throughout euchromatin.

In the scope of multi-institutional collaboration, we participated in the study of the evolution of molecular resistance of vertebrates to snake venom α-neurotoxins (M.A. Khan et al., *Toxins*, 12 (2020), 638). These toxins bind to nicotinic acetylcholine receptor (nAChR) at the neuromuscular junction, causing muscle paralysis that leads to suffocation. Several venomous snakes and their predators have, however, evolved resistance to such toxins. The resistance is due to a steric hindrance between glycosylated Asn at positions 187 or 189 in the nAChR ligand-binding domain and α-neurotoxins, by electrostatic repulsion or steric hindrance between positively charged α-neurotoxins and the Arg187 of the nAChR. The inhibition of the α-neurotoxins binding to nAChR can also be due to structural changes of the receptor induced by Pro194 or Pro197 replacement. We analysed the nAChR ligand-binding domain of 148 vertebrate species, and assessed their amino acid sequences for the resistance-associated mutations. We found a widespread convergent evolution of the *N*-glycosylation form of resistance in several taxa, including venomous snakes and their lizard preys, but not in the snake-feeding birds. We also documented new lineages with the Arg form of inhibition. Using an *in vivo* assay in four species, we provided further evidence that *N*-glycosylation mutations of nAChR reduce the toxicity of cobra venom. Our research shows that the evolution of α-neurotoxins in snakes may well have prompted arms races and mutations to this ancient receptor across a wide range of vertebrates (Figure 5).

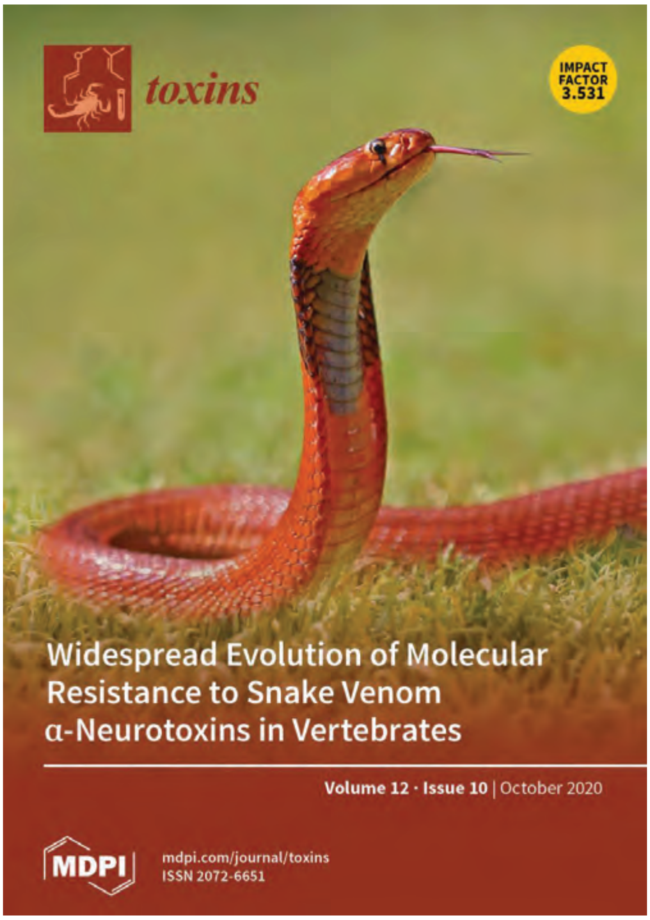

Figure 5: Another example of our work was highlighted on the cover page, this time of the October issue of Toxins. In our paper inside, we showed that the resistance to snake venom α-neurotoxins occurred by impairing the binding of these toxins to the nicotinic acetylcholine receptor (nAChR) attained in the process of its convergent evolution. The resistance is due to mutation that results in the attachment of a branched glycan chain to a specific Asn in the ligand-binding region of nAChR. This N-glycosylation then, sterically or electrostatically, prevents binding of α-neurotoxins, large snake venom peptides, to nAChR whereas the binding of a small endogenous neurotransmitter ACh remains normal. We established that the convergent evolution of the resistance to α-neurotoxins by N-glycosylation of nAChR is widespread in vertebrates.

Other subjects

We also participated in several research projects out of the thematic scope of our department. Two such collaborations resulted in publications in 2020.

Participating with fluorescence microscopy analysis, we co-authored a paper in which we studied glioblastoma, a particularly common and very aggressive primary brain tumour (A. Zottel et al., *Ther. Adv. Med. Oncol.*, 12 (2020), 1758835920915302). One of the main causes of therapy failure is the presence of glioblastoma stem cells that are resistant to chemotherapy and radiotherapy, and that have the potential to form new tumours. Our study was focused on the validation of eight novel antigens, TRIM28, nucleolin, vimentin, NAP1L1, TUFM, DPYSL2, CRMP1 and ALYREF, as putative glioblastoma targets, using nanobodies. Indicated for further examination, cells have been exposed to anti-vimentin, anti-NAP1L1, anti-TUFM or anti-DPYSL2 nanobodies. Therapeutically, the most interesting effects were demonstrated using anti-TUFM and anti-vimentin nanobodies. The former induced a potent inhibition of glioblastoma cell growth after long-term exposure, having only minor effects on astrocytes. The latter efficiently inhibited cell migration.

In the scope of the ARRS applicative project L4-1839, led by the colleagues from the Biotechnical Faculty of the University of Ljubljana, we participated at preparing of a review paper on the most distinct properties of chestnut honey, important for its medical application (J. Božič et al., *Acta Biol. Slov.*, 62 (2020), 31–44).

As partners in the ARRS project J7-7424, led by colleagues from the Faculty of Electrical Engineering at the University of Ljubljana, we participated with the analysis of nanoparticles' protein corona composition to explain their cytotoxicity and induction of cytokine secretion in THP-1 macrophages. At the end of 2020, the paper was submitted for publication in the prestigious journal *Small* (K. Strojan et al., submitted).

Also, in the field of nanoparticles research, this time in collaboration with our partners from the Ruđer Bošković Institute in Zagreb, we participated in establishing the mechanism of formation and morphogenesis of *Arca noae* shell's nanoscale biomineral structures. We accomplished the mass-spectrometric identification of protein components of the shell, potentially involved in the process of biomineralization, i.e., initiation of the extracellular nucleation of aragonite nanocrystals. The paper was prepared and is currently under peer review in *J. Colloid Interface Sci.* (V. Čadež et al., submitted).

In 2020 we started the collaboration on three novel ARRS research projects. As experts on proteomics, we are involved in study J3-2521 of the inflammatory process in interstitial cystitis and an evaluation of the influence of cannabinoid receptor agonists in the urinary bladder (leading institution: the Medical Faculty at the University of Ljubljana). As partners in the project J1-2482 (leading institution: BF/UL), we are participating at assessment of impact of environmentally relevant nano- and micro-plastics on soil invertebrates, while as partners in the project J1-2469 (leading institution: BF/UL), we are contributing at analysis of genomic and transcriptomic data to deepen insight into the exceptional biology of proteus (*Proteus anguinus*).

Following the covid-19 pandemic outbreak, we initiated research on SARS-CoV-2. The first aspect of these studies is genomic analysis and molecular evolution of SARS-CoV-2 and other coronaviruses, with the aims to characterize the evolutionarily constrained regions of the pathogen genome, which should be preferentially targeted to avoid rapid drug-resistant mutants, and to identify viral genes interacting with those of its host. Stemming from the latter, we have been working on the integrative genomics of SARS-CoV-2 in human cells, specifically by analysing the binary protein-protein interactions of viral and human proteins. Based on the results of this research, the physiological effects of selected SARS-CoV-2 proteins on cultured human cells will be investigated to validate the functional relevance of the interactions between viral proteins or their variants and their corresponding human protein targets.

Some outstanding publications in the past year

1. Latinović, Z., Leonardi, A., Koh, C.Y., Kini, R.M., Trampuš Bakija, A., Pungerčar, J. and Križaj, I.: The procoagulant snake venom serine protease potentially having a dual, blood coagulation factor V and X-activating activity. Toxins, 12 (2020), 358
2. Lang Balija M., Leonardi, A., Brgles, M., Sviben, D., Kurtović, T., Halassy, B. and Križaj, I.: Biological activities and proteomic profile of the venom of *Vipera ursinii* ssp., a very rare karst viper from Croatia. Toxins, 12 (2020), 187
3. Ha, V.T., Lainšček, D., Gesslbauer, B., Jarc-Jovičić, E., Hyötyläinen, T., Ilc, N., Lakota, K., Tomšič, M., van de Loo, F.A.J., Bochkov, V., Petan, T., Jerala, R. and Manček-Keber, M.: Synergy between 15-lipoxygenase and secreted PLA_2 promotes inflammation by formation of TLR4 agonists from extracellular vesicles. Proc. Natl. Acad. Sci. USA, 117 (2020), 25679–25689
4. Ott Rutar, S. and Kordiš, D.: Analysis of the RNA virome of basal hexapods. Peer J., 8 (2020), e8336
5. Jarc, E. and Petan, T.: A twist of FATe: lipid droplets and inflammatory lipid mediators. Biochimie, 169 (2020), 69–87

Awards and appointments

1. Sabina Drofenik: Prešeren Prize for Students of the University of Ljubljana 2020, University of Ljubljana, award-wining bachelor's thesis entitled Description of the mechanism and interdependence of the ac-

tion of two nose-horned viper venom proteins, secretory phospholipase A_2 and chymotrypsin inhibitor (co-mentor Prof. Dr. Igor Križaj)

2. Eva Jarc Jovičić: 50th Krka Prizes, Krka recognition with special honours for the research work, Krka d.d., for the doctoral thesis entitled The role of lipid droplets in cancer cell stress resistance
3. Zorica Latinović: 50th Krka Prizes, Krka recognition with special honours for the research work, Krka d.d., for the doctoral thesis entitled Components of the nose-horned viper venom that affect cardiovascular system
4. Adrijana Leonardi, Kity Požek, Igor Križaj: 7th International Toxinology Meeting, Poster Award for the poster entitled Biochemical and functional characterization of the first member of the new P-IIIe subclass of snake venom metalloproteinases
5. Primož Godec, Matjaž Pančur, Nejc Ilenič, Andrej Čopar, Martin Stražar, Aleš Erjavec, Ajda Pretnar, Janez Demšar, Anže Starič, Marko Toplak, Lan Žagar, Jan Hartman, Hamilton Wang, Riccardo Bellazzi, Uroš Petrovič, Silvia Garagna, Maurizio Zuccotti, Dongsu Park, Gad Shaulsky, Blaž Zupan: Best Research Achievements of the University of Ljubljana 2020, University of Ljubljana, for publication: Democratized image analytics by visual programming through integration of deep models and small-scale machine learning, Nature Communications 10 (2020): 4551.

INTERNATIONAL PROJECT

1. Do Endogenous Secreted Phospholipases A2 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. DNA sampling II: a method for identification of directly or indirectly bound proteins at specific loci on bacterial chromosomes
   Prof. Igor Križaj
2. Neurotoxicity or neuroprotection of nanomaterials: the rele of biocorona
   Prof. Igor Križaj
3. Protein complexes from the fungal genus Pleurotus, new biopesicides for controlling Colorado potato beetle and western corn rootworm
   Prof. Igor Križaj
4. Exploitation of a virus-borne small protein to combat antibiotic resistance in Staphylococcus aureus
   Prof. Igor Križaj
5. Genomic and transcriptomic insights into the exceptional biology of proteus (Proteus anguinus)
   Prof. Dušan Kordiš
6. Impact of environmentally relevant nano- and micro-plastics on soil invertebrates
   Prof. Igor Križaj
7. Inflammatory process in interstitial cystitis and evaluation of the influence of cannabinoid receptor agonists in urinary bladder - from cells to patients
   Prof. Igor Križaj
8. „Reversibility of transient thrombocytopenia induced by a snake venom component offers asafe antithrombotic prevention in interventional angiology and cardiology“
   Prof. Igor Križaj
9. Bisphenol A alternatives: transfer from food contact material, fate and human exposure
   Prof. Toni Petan
10. Anisotropic magnetic nanoparticles for the magneto-mechanical therapy of cancer
    Prof. Igor Križaj
11. Neuropsychological dysfunctions caused by low level exposure to selected environmental pollutants in susceptible population – NEURODYS
    Prof. Igor Križaj
12. Targeting lipid droplets to reduce cancer cell resistance to stress
    Prof. Toni Petan
13. Development of an innovative drug to treat venous thromboembolism based on a unique viper venom anticoagulant
    Prof. Igor Križaj
14. Development of medical chestnut honey quality control and technology
    Prof. Igor Križaj

STAFF

Researchers
1. Prof. Dušan Kordiš
2. **Prof. Igor Križaj, Head**
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4. Prof. Toni Petan
5. Prof. Uroš Petrovič*
6. Prof. Jože Pungerčar
7. Dr. Jernej Šribar

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9. Dr. Mojca Ogrizović
10. Dr. Nina Zupanič

Postgraduates
11. Tadeja Bele, B. Sc.
12. Adrijan Ivanušec, B. Sc.
13. Ana Kump, B. Sc.
14. Gašper Žun, B. Sc.

Technical officer
15. Kity Požek, B. Sc.

Technical and administrative staff
16. Igor Koprivec
17. Maja Šimaga, M. Sc.

Note:

* part-time JSI member

BIBLIOGRAPHY

Original Article

1. Sabina Ott Rutar, Dušan Kordiš, "Discovery and molecular characterisation of the first ambidensovirus in honey bees", *Acta agriculturae Slovenica*, 2020, **116**, 2, 383-393.
2. Janko Božič, Jasna Bertoncelj, Damjana Drobne, Gordana Glavan, Nina Gunde-Cimerman, Adrijana Leonardi, Rok Kopinč, Anita Jemec Kokalj, Sara Novak, Mojca Korošec, Igor Križaj, Blaž Podrižnik, Martina Turk, Andrej Zabret, "The quality of Slovenian chestnut honey and its specific properties relevant for medical application and functional nutrition", *Acta biologica slovenica: ABS*, 2020, **63**, 2, 31-44.
3. Federica Valdetara, Miha Škalič, Daniela Fracassetti, Marli Louw, Concetta Compagno, Maret Du Toit, Roberto Foschino, Uroš Petrovič, Benoit Divol, Ileana Vigentini, "Transcriptomics unravels the adaptive molecular mechanisms of *Brettanomyces bruxellensis* under SO_2 stress in wine condition", *Food microbiology*, 2020, **90**, 103483.
4. Isidoro Feliciello, Željka Pezer, Dušan Kordiš, Branka Bruvo Mađarić, Đurđica L. Ugarković, "Evolutionary history of alpha satellite DNA repeats dispersed within human genome euchromatin", *Genome biology and evolution*, 2020, **12**, 11, 2125-2138.
5. Alja Zottel, Neja Šamec, Ana Kump, Lucija Raspor Dall'Olio, Pia Pužar Dominkuš, Rok Romih, Samo Hudoklin, Jernej Mlakar, Daniil Nikitin, Maxim Sorokin, Anton A. Buzdin, Ivana Jovchevska, Radovan Komel, "Analysis of miR-9-5p, miR-124-3p, miR-21-5p, miR-138-5p, and miR-1-3p in glioblastoma cell lines and extracellular vesicles", *International journal of molecular sciences*, 2020, **21**, 22, 8491.
6. Nina Zupanič, Hristo Hristov, Matej Gregorič, Urška Blaznik, Nataša Delfar, Barbara Koroušić-Seljak, Eric L. Ding, Nataša Fidler Mis, Igor Pravst, "Total and free sugars consumption in a Slovenian population representative sample", *Nutrients*, 2020, **12**, 6, 1729.
7. Sabina Ott Rutar, Dušan Kordiš, "Analysis of the RNA virome of basal hexapods", *PeerJ*, 2020, **8**, c8336.
8. Van Thai Ha, Duško Lainšček, Bernd Gesslbauer, Eva Jarc Jovičić, Tuulia Hyötyläinen, Nejc Ilc, Katja Lakota, Matija Tomšič, Fons A. J. Van de Loo, Valery Bochkov, Toni Petan, Roman Jerala, Mateja Manček Keber, "Synergy between 15-lipoxygenase and secreted PLA_2 promotes inflammation by formation of TLR4 agonists from extracellular vesicles", *Proceedings of the National Academy of Sciences of the United States of America*, 2020, **117**, 41, 25679-25689.
9. Alja Zottel, Ivana Jovchevska, Neja Šamec, Jernej Mlakar, Jernej Šribar, Igor Križaj, Marija Skoblar Vidmar, Radovan Komel, "Anti-vimentin, anti-TUFM, anti-NAP1L1 and anti-DPYSL2 nanobodies display cytotoxic effect and reduce glioblastoma cell migration", *Therapeutic advances in medical oncology*, 2020, **12**, 1-29.
10. Sabina Drofenik, Adrijana Leonardi, Monika C. Žužek, Robert Frangež, Igor Križaj, "The first Kunitz-type proteins from a viperid venom that potentiate neuromuscular transmission", *Toxicon*, 2020, **187**, 262-270.
11. Maja Lang Balija, Adrijana Leonardi, Marija Brgles, Dora Sviben, Tihana Kurtović, Beata Halassy, Igor Križaj, "Biological activities and proteomic profile of the venom of *vipera ursinii* ssp., a very rare Karst viper from Croatia", *Toxins*, 2020, **12**, 3, 187.
12. Zorica Latinović, Adrijana Leonardi, Cho Yeow Koh, R. Manjunatha Kini, Alenka Trampuš-Bakija, Jože Pungerčar, Igor Križaj, "The procoagulant snake venom serine protease potentially having a dual, blood coagulation factor V and X-activating activity", *Toxins*, 2020, **12**, 6, 358.
13. Muzaffar A. Khan *et al.* (13 authors), "Widespread evolution of molecular resistance to snake venom α-neurotoxins in vertebrates", *Toxins*, 2020, **12**, 10, 638.

Review Article

1. Eva Jarc, Toni Petan, "A twist of FATe: lipid droplets and inflammatory lipid mediators", *Biochimie*, 2019, **169**, 69-87.

Independent Component Part or a Chapter in a Monograph

1. Nina Zupanič, Nataša Fidler Mis, Igor Pravst, "Soft drinks: public health perspective", In: *Trends in non-alcoholic beverages*, Academic Press, 2020, 325-369.

Theses and Mentoring

1. Zorica Latinović, *Components of the nose-horned viper venom that affect cardiovascular system:* doctoral dissertation, Ljubljana, 2020 (mentor Igor Križaj; co-mentor Adrijana Leonardi).
2. Nina Zupanič, *Sugar in pre-packaged foods and in diet among children in Slovenia:* doctoral dissertation, Ljubljana, 2020 (mentor Nataša Fidler Mis; co-mentor Igor Pravst).

DEPARTMENT OF BIOTECHNOLOGY
B-3

At the Department of Biotechnology we investigate biological molecules of animal, plant microbiological, fungal and origin using modern biotechnological methods. We would like to apply them for diagnostic and therapeutic purposes in human and veterinary medicine, for plant protection, the preparation of high-quality and safe food and for the protection of the environment, contributing to an improvement of peoples' health and 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 on the role of cysteine peptidases and their inhibitors in the regulation of an anti-tumour immune response. Besides the important role of these enzymes and inhibitors in the function of natural killer cells, as demonstrated by our group in previous years, we showed their important function also for cytotoxic T cells. Cytotoxic T lymphocytes kill cancer or virally infected cells by exocytosis of the lytic granules. This leads to perforin-mediated granzyme entry into the target cell, consequently killing the target cell. Granzymes and perforin are activated by cysteine cathepsins, whose activity is regulated by the protein inhibitor cystatin F. Since cystatin F can be secreted by a range of cancer and immune cells in tumour micro-environments, we investigated whether extracellular cystatin F can be taken up by and affect the function of cytotoxic T lymphocytes. We demonstrated cystatin F uptake into cytotoxic T lymphocytes, the down-regulation of target peptidases, and reduced target cell killing. Overall, our results indicate that cystatin F is an important mediator that can impair the killing efficiency of cytotoxic T lymphocytes and thus suggest that it is a possible target for cancer immunotherapy.

Extracellular cystatin F is internalised by cytotoxic T lymphocytes and decreases their cytotoxicity

Molecular neurodegeneration

With the aging population and lack of 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 (TDP-43, FUS, C9orf72, SFPQ, MATR3, etc.) associated with amyotrophic lateral sclerosis (ALS), frontotemporal dementia (FTD) and Alzheimer's disease (AD). The majority of these genes are in some way associated with RNA biogenesis, processing, transport and turnover. We study nuclear transport, cellular stress response and macromolecular interactions, leading to the mislocalization and aggregation of these proteins. In 2020 we created a cell line that can be used to measure stress granule formation, which is one of the ways cells deal with acute stress response and, besides validating the cells with standard cellular stressors, we showed that cold atmospheric plasma can also cause a transient stress response in cells. We advanced our interactomic studies of TDP-43, FUS and dipeptide repeats from C9orf72 mutation finding mechanistically and pathologically important interactors for all. In collaboration with the Veterinary Faculty, University of Ljubljana, we have studied nitrosative stress in canine cognitive dysfunction (CCD), which is an age-related disorder that occurs in elderly dogs with similarities to Alzheimer's disease. We reported that neuro-inflammation and nitrosative stress that we observed in CCD-affected brains can exacerbate the neurodegenerative process ultimately leading to cognitive impairment.

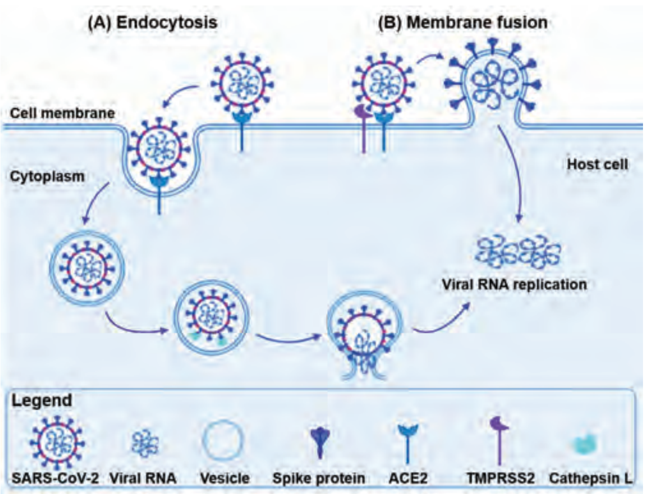

Figure 1:Mechanisms of entry of SARS-CoV-2 to host cells

As the Slovenian lead of the global genetic consortia for the determination of genetic causes of ALS (Project MiNE) and FTD (IFGC), we were involved in three published studies. With a population genetic analysis of FTD cohorts we showed that the C9orf72 mutation, age at onset of the disease, and ancestry can help discriminate between behavioural language variants of FTD. On the ALS genetics front we studied the shared common genetic risk of amyotrophic lateral sclerosis and epilepsy and reported that that the risk is not shared and that hyper-excitability in both diseases has different origins.

Prader Willi syndrome and RNA biology

Prader Willi syndrome is a rare metabolic and neurological developmental disorder, where dysregulation of a genomic region that caries SNORD116 snoRNA cluster leads to the disease. With the aim of finding therapeutical targets, we are using RNA-RNA interactomics to determine the interactors of SNORD116 and have managed to create four independent libraries from two cell lines, which will be analysed in 2021. At the beginning of 2020 we also published a review on noncanonical functions of snoRNAs in the reputable journal Nucleic Acids Research (IF=11.1).

L. lactis can serve as a carrier in targeted drug delivery when coupled to a therapeutic moiety

Probiotics

At the department we continued our work on probiotic lactic acid bacteria. We have prepared a review of the studies of the influence of probiotics on the Firmicutes/Bacteroidetes ratio and its consequence for the treatment of obesity and inflammatory bowel disease. We have also continued our collaboration with the Chair of Pharmaceutical Technology from the Faculty of Pharmacy in incorporating four probiotic vaginal lactobacilli in nanofibers for the development of potential new delivery system. To facilitate the monitoring of the incorporation and release of lactobacilli, we labelled different species of lactobacilli with different fluorescent proteins by using genetic engineering. This enabled the straightforward identification and tracking of individual species. Additionally, we prepared a thorough review of the use of electrospun nanofibers as carriers of micro-organisms, as well as of biologically relevant molecules, such as proteins and nucleic acids, demonstrating the feasibility of electrospinning of sensitive biological components.

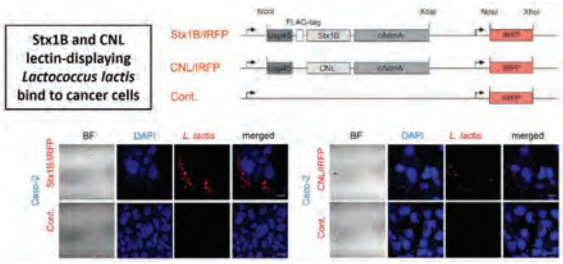

Figure 2: L. lactis genetic constructs for surface display of lectins Stx1B and CNL (above), and demonstration of specific binding of these engineered bacteria to Caco-2 cancer cells (below).

We have also continued with our work on the genetic engineering of lactic acid bacteria as the tool for the delivery of biotherapeutics, focusing on their application in our project of treating colorectal cancer. Lectins have been increasingly utilized as carriers for targeted drug delivery based on their specific binding to glycans located on mammalian cells. We engineered *L. lactis* to display two lectins, Stx1B and CNL, on its surface and concomitantly express fluorescent protein for detection. We verified the presence of lectins´ target sites on HeLa, HT-29 and Caco-2 cells and demonstrated the lectin-mediated adhesion of engineered bacteria to these cells. Thus, lectin-displaying *L. lactis* might serve as a carrier in targeted drug delivery when coupled to a therapeutic moiety. The safety and regulatory acceptance of engineered lactic acid bacteria is a frequent issue with regard of the low public acceptance of genetically modified organisms. We have addressed different aspects of this issue in detail in another review paper published in 2020.

Glycobiology

In the field of glycobiology, in 2020 we continued with research focused on the molecular mechanisms of bacterial biofilm development. In cooperation with the Biotechnical Faculty of the University of Ljubljana, we showed that glycans in the bacterial surfactome affect the adhesion of bacteria to surfaces and can therefore be used as target molecules to prevent bacterial adhesion. The adhesion of the bacterium to the surface represents the first step in the formation of biofilms that allow the bacteria to survive in adverse conditions, and thus cause recurrent and persistent infections. Preventing biofilm formation through alternative approaches is an important strategy to reduce antibiotic use. We further developed a new method for monitoring the development of listeria biofilms based on bioluminescence. Namely, we expressed the highly efficient NanoLuc luciferase in *Listeria innocua* and showed that the bioluminescence-based test allows direct detection, absolute cell quantification, broad dynamic range, and high sensitivity. The new test represents a good alternative or complement to the existing methods of biofilm quantification.

We created a cell line that can be used to measure stress granule formation and screen for therapeutics that regulate cellular response to stress.

COVID-19

Within a new project on research and treatment of the Covid-19 pandemic, approved by Slovenian Research Agency in 2020, we started to investigate the role of viral and host peptidases in cell entry and replication of SARS-CoV-2. In these processes in particular cysteine peptidases are important; therefore, we explored a large library of small synthetic inhibitors developed by our group for other different purposes. In collaboration with colleagues from International Centre of Genetic Engineering (ICGEB) from Trieste, Italy, we showed that inhibitors, specific to cathepsin B and possessing quinoline structure, effectively prevent SARS-CoV-2 replication. One of these compounds is nitroxoline, an established antibiotic, which we intend to evaluate as a potential antiviral drug in preclinical and clinical studies. The use of cysteine peptidase inhibitors as potential antiviral drugs was included in the international patent application.

The results of the research work at the Department of Biotechnology in 2019 were published in 34 scientific papers in journals with an impact factor. We received two new research grants from the Slovenian Research Agency. Prof. Boris Rogelj received the national Zois recognition for scientific achievements in molecular basis of neurodegeneration, Nika Kruljec and Katja Škrlec received Krka awards and Abida Zahirović received the Dean's Award from the Faculty of Pharmacy. Members of the department were also very active in pedagogical work as lecturers and mentors to students preparing diploma and doctoral thesis at the universities in Slovenia and abroad. In 2019 two doctoral theses were completed at the department.

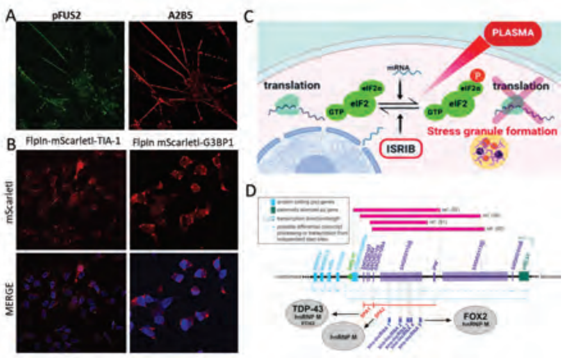

Figure 3: Mechanisms associated with neurological disorders ALS, FTD and PWS. A) expression of phosphorylated FUS (green) in astrocytes stained with A2B5 (red) marker. B) Stress granule formation visualized with markers TIA-1 and G3BP1 (red). C) Mechanism of stress granule formation induced by cold atmospheric plasma. D) Genomic region associated with PWS and RNA binding proteins that may influence expression from the region.

Some outstanding publications in the past year

1. Costa, Beatriz, et al., For the International FTD-Genetics Consortium (IFGC). C9orf72, AAO and ancestry help discriminating behavioural from language variants in FTLD cohorts. *Neurology*, ISSN 0028-3878, [in press] 2020, 41 str., doi: 10.1212/WNL.0000000000010914. [COBISS.SI-ID 29979139]
2. Bratkovič, Tomaž, Božič, Janja, Rogelj, Boris. Functional diversity of small nucleolar RNAs. *Nucleic acids research*, ISSN 0305-1048, Feb. 2020, vol. 48, issue. 4, str. 1627-1651, ilustr. https://academic.oup.com/nar/article/48/4/1627/5673630?guestAccessKey=0bc2e46c-b45c-4562-81be-8137020800a3, doi: 10.1093/nar/gkz1140. [COBISS.SI-ID 4860017]
3. Plavec, Tina Vida, Berlec, Aleš. Safety aspects of genetically modified lactic acid bacteria. *Microorganisms*. 2020, vol. 8, no. 2, str. 297-1-297-21. ISSN 2076-2607. DOI: 10.3390/microorganisms8020297. [COBISS.SI-ID 33217063]
4. Pišlar, Anja, Mitrović, Ana, Sabotič, Jerica, Pečar Fonović, Urša, Perišić, Milica, Jakoš, Tanja, Senjor, Emanuela, Kos, Janko. The role of cysteine peptidases in coronavirus cell entry and replication : the therapeutic potential of cathepsin inhibitors. *PLOS pathogens*. 2020, vol. 16, no. 11, str. 1-3, https://journals.plos.org/plospathogens/article/file?id=10.1371/journal.ppat.1009013&type=printable, DOI: 10.1371/journal.ppat.1009013. [COBISS.SI-ID 36092931]
5. Prunk, Mateja, Perišić, Milica, Jakoš, Tanja, Sabotič, Jerica, Švajger, Urban, Kos, Janko. Extracellular cystatin F is internalised by cytotoxic T lymphocytes and decreases their cytotoxicity. *Cancers*. Dec. 2020, vol. 12, iss. 12, str. 1-14, ilustr. ISSN 2072-6694. https://www.mdpi.com/2072-6694/12/12/3660, DOI: 10.3390/cancers12123660. [COBISS.SI-ID 43955203]

Awards and Appointments

1. Jernej Birk, Domen Hočevar, Kaja Rangus: Krka Award for undergraduate research assignments, Krka, d.d., Use of microthermophoresis to determine sugar binding to rCnSL-B2 isolectin (Mentors: Janja Pust, dr. Jerica Sabotič, dr. Ana Mitrović)
2. Urša Čerček: Faculty of Pharmacy student Prešeren award 2020, Ljubljana, Faculty of Pharmacy, Effect of cold atmospheric pressure plasma on formation of stress granules in the selected stable cell line.
3. Urša Čerček: Krka recognition for undergraduate and postgraduate research work, Krka, Effect of cold atmospheric pressure plasma on formation of stress granules in the selected stable cell line.
4. Neja Kuret: Krka Award, Krka, d.d., Effect of kokaprin lectin on pathogenic and probiotic bacteria (Mentors: doc. dr. Anja Klančnik, dr. Jerica Sabotič)
5. Mirjana Malnar: Award for presentation of research achievements in terms of scientific quality and their applicability, 12th Jožef Stefan International Postgraduate School Students' Conference and 14th CMBE day, presentation of research work
6. Emanuela Senjor: 3rd place UCLA Research Day 2020 Poster Competition, Los Angeles, USA, University of California Los Angeles, School of Dentistry

INTERNATIONAL PROJECTS

1. De-regulated expression of CodY controlled proteins in L. lactis for enhancing nisin production
   Prof. Aleš Berlec
   Fermentech Gsv Pvt Ltd.
2. COST CA18238; Ocean4Biotech - European Transdisciplinary Networking Platform for Marine Biotechnology
   Dr. Jerica Sabotič
   Cost Association Aisbl
3. COST CA19123 - PHOENIX; Protection, Resilience, Rehabilitation of Damaged Environment
   Prof. Aleš Berlec
   Cost Association Aisbl
4. Neuropathological Evaluation of the In Vivo Interactomes of TDP-43, FUS and MATR3 in Human ALS and FTD
   Slovenian Research Agency
   Prof. Boris Rogelj
5. Crosstalk of Proteinopathy and Inflammation in Amyotrophic Lateral Sclerosis
   Slovenian Research Agency
   Prof. Boris Rogelj

RESEARCH PROGRAMME

1. Pharmaceutical Biotechnology: Knowledge for Health
   Prof. Janko Kos

R & D GRANTS AND CONTRACTS

1. Nucleart transport defect in neurodegenerative diseases
   Prof. Boris Rogelj
2. Cathepsin X inhibitors impair the resistence of tumor cells to antiprotease therapy
   Prof. Janko Kos
3. Pathogenic role of paraspeckle-like nuclear bodies in neurodegenerative diseases ALS and FTD
   Prof. Boris Rogelj
4. Inhibition of cathepsin X activity as a novel strategy for the treatment of Parkinson's disease
   Prof. Janko Kos
5. Targeting Campylobacter adhesion in the fight against antimicrobial resistance
   Dr. Jerica Sabotič
6. Targeting, imaging and treating of colorectal cancer with safe theranostic bacteria
   Prof. Aleš Berlec
7. Phase transitions in systems of nucleotide repeat expansions associated with neurodegenerative diseases
   Prof. Boris Rogelj
8. New antimicrobial strategies in prevention of biofilm formation by using lectins that inhibit bacterial adhesion
   Dr. Jerica Sabotič
9. Improvement of immunotherapeutic potential of NK cells through modulation of cystatin F
   Prof. Janko Kos
10. Nuclear transport defects in frontotemporal dementia
    Prof. Boris Rogelj
11. Cystatin f as a mediator of immunosuppression in glioblastoma microenvironment
    Dr. Milica Perišić Nanut
12. FunContrAPest: Novel Fungal Proteins as Biopesticides for Control of Challenging Invasive Alien Agricultural Pests
    Dr. Jerica Sabotič
13. Innovative ECO plasma seed treatment (for sowing and for human and animal diet/nutrition
    Prof. Boris Rogelj
    Ministry of Education, Science and Sport
14. Bacterial Cell Wall Glycans
    Dr. Jerica Sabotič
    Institut De Biologie Structurale

STAFF

Researchers
1. Prof. Aleš Berlec
2. Prof. Janko Kos*
3. Asst. Prof. Helena Motaln
4. **Prof. Boris Rogelj, Head**
5. Dr. Jerica Sabotič
6. Prof. Borut Štrukelj*

Postdoctoral associates
7. Dr. Janja Božič
8. Dr. Nikolaja Janež
9. Dr. Ana Mitrović
10. Dr. Eva Ogorevc
11. Dr. Milica Perišić Nanut
12. Dr. Mateja Prunk
13. *Dr. Anja Pucer Janež, left 01.03.20*
14. Dr. Abida Zahirović

Postgraduates
15. Urša Čerček, B. Sc.
16. *Mirjana Malnar, B. Sc., left 01.10.20*
17. Tina Vida Plavec, B. Sc.
18. Emanuela Senjor, B. Sc.

Technical officer
19. *Eva Erzar, B. Sc., left 01.10.20*

Technical and administrative staff
20. Maja Šimaga, M. Sc.

Note:

* part-time JSI member

BIBLIOGRAPHY

Original Article

1. Helena Motaln, Urša Čerček, Nina Recek, Ana Bajc Česnik, Miran Mozetič, Boris Rogelj, "Cold atmospheric plasma induces stress granule formation *via* an eIF2α-dependent pathway", *Biomaterials science*, 2020, **8**, 19, 5293-5305.
2. Tanja Jakoš, Anja Pišlar, Urša Pečar Fonović, Urban Švajger, Janko Kos, "Cysteine cathepsins L and X differentially modulate interactions between myeloid-derived suppressor cells and tumor cells", *Cancer immunology and immunotherapy*, 2020, **69**, 1869-1880.
3. Mateja Prunk, Milica Perišić, Tanja Jakoš, Jerica Sabotič, Urban Švajger, Janko Kos, "Extracellular cystatin F is internalised by cytotoxic T lymphocytes and decreases their cytotoxicity", *Cancers*, 2020, **12**, 12, 3660.
4. Teja Lavrin, Tilen Konte, Rok Kostanjšek, Simona Sitar, Kristina Sepčić, Sonja Prpar Mihevc, Ema Žagar, Vera Župunski, Metka Lenassi, Boris Rogelj, Nina Gunde-Cimerman, "The neurotropic black yeast Exophiala dermatitidis induces neurocytotoxicity in neuroblastoma cells and progressive cell death", *Cells*, 2020, **9**, 4, 963.
5. Ana Bajc Česnik, Helena Motaln, Boris Rogelj, "The impact of ALS-associated genes hnRNPA1, MATR3, VCP and UBQLN2 on the severity of TDP-43 aggregation", *Cells*, 2020, **9**, 8, 1791.
6. Tim Van de Walle *et al.* (14 authors), "Synthesis of novel nitroxoline analogs with potent cathepsin B exopeptidase inhibitory activity", *ChemMedChem*, 2020, **15**, 24, 2477-2490.
7. Anahid Jewett, Janko Kos, Kawaljit Kaur, Tamara Lah Turnšek, Barbara Breznik, Emanuela Senjor, Paul Wong, Kristin Y. Nguyen, Meng-Wei Ko, "Multiple defects of natural killer cells in cancer patients: anarchy, dysregulated systemic immunity, and immunosuppression in metastatic cancer", *Critical reviews in immunology*, 2020, **40**, 2, 93-133.
8. Urša Pečar Fonović, Damijan Knez, Martina Hrast, Nace Zidar, Matic Proj, Stanislav Gobec, Janko Kos, "Structure-activity relationships of triazole-benzodioxine inhibitors of cathepsin X", *European Journal of Medicinal Chemistry*, 2020, **193**, 112218.
9. Urban Košak, Nika Strašek, Damijan Knez, Marko Jukič, Simon Žakelj, Abida Zahirović, Anja Pišlar, Xavier Brazzolotto, Florian Nachon, Janko

Kos, Stanislav Gobec, "N-alkylpiperidine carbamates as potential anti-Alzheimer's agents", *European Journal of Medicinal Chemistry*, 2020, **197**, 112282.
10. Saša Haberl Meglič, Nikolaja Janež, Matjaž Peterka, Karel Flisar, Tadej Kotnik, Damijan Miklavčič, "Evaluation and optimization of protein extraction from *E. coli* by electroporation", *Frontiers in bioengineering and biotechnology*, 2020, **8**, 543187.
11. Ana Rotter *et al.* (51 authors), "A new network for the advancement of marine biotechnology in Europe and beyond", *Frontiers in marine science*, 2020, **7**, 278.
12. Jerica Sabotič, Jože Brzin, Jana Erjavec, Tanja Dreo, Magda Tušek-Žnidarič, Maja Ravnikar, Janko Kos, "L-amino acid oxidases from mushrooms show antibacterial activity against the phytopathogen *Ralstonia solanacearum*", *Frontiers in microbiology*, 2020, **11**, 977-1-997-18.
13. Anja Pišlar, Larisa Tratnjek, Gordana Glavan, Nace Zidar, Marko Živin, Janko Kos, "Neuroinflammation-induced upregulation of glial cathepsin X expression and activity in vivo", *Frontiers in molecular neuroscience*, 2020, **13**, 224.
14. Sonja Prpar Mihevc, Maja Zakošek, Malan Štrbenc, Boris Rogelj, Gregor Majdič, "Nitrosative stress in the frontal cortex from dogs with canine cognitive dysfunction", *Frontiers in veterinary science*, 2020, **7**, 573155, 916.
15. Damijan Knez, Natalia Colettis, Luca G. Iacovino, Matej Sova, Anja Pišlar, Janez Konc, Samo Lešnik, Josefina Higgs, Fabiola Kamecki, Irene Mangialavori, Ana Dolšak, Simon Žakelj, Jurij Trontelj, Janko Kos, Claudia Binda, Nora Marder Mariel, Stanislav Gobec, "Stereoselective activity of 1-propargyl-4-styrylpiperidine-like analogues that can discriminate between monoamine oxidase isoforms A and B", *Journal of medicinal chemistry*, 2020, **63**, 3, 1361-1387.
16. Tim Božič, Matja Zalar, Boris Rogelj, Janez Plavec, Primož Šket, "Structural diversity of sense and antisense RNA hexanucleotide repeats associated with ALS and FTLD", *Molecules*, 2020, **25**, 3, 525.
17. Kaja Rožman, Evan M. Alexander, Eva Ogorevc, Krištof Bozovičar, Izidor Sosič, Courtney C. Aldrich, Stanislav Gobec, "Psoralen derivatives as inhibitors of mycobacterium tuberculosis proteasome", *Molecules*, 2020, **25**, 6, 1305.
18. Mateja Sirše, Samo K. Fokter, Borut Štrukelj, Janja Zupan, "Silver fir (*Abies alba L.*) polyphenolic extract shows beneficial influence on chondrogenesis in vitro under normal and inflammatory conditions", *Molecules*, 2020, **25**, 20, 4616.
19. Damijan Knez, Izidor Sosič, Ana Mitrović, Anja Pišlar, Janko Kos, Stanislav Gobec, "8-hydroxyquinoline-based anti-Alzheimer multimodal agents", *Monatshefte für Chemie*, 2020, **151**, 1111-1120.
20. Beatriz Costa *et al.* (109 authors), For the International FTD-Genetics Consortium (IFGC), "C9orf72, AAO and ancestry help discriminating behavioural from language variants in FTLD cohorts", *Neurology*, 2020, **95**, 24, e3288-e3302.
21. Tanja Gmeiner, Jasna Grželj, Borut Štrukelj, Luka Stopar, Pij B. Marko, "Psoriasis: a comprehensive review on the aetiopathogenesis and recent advances in long-term management of patients with plaque psoriasis", *Pharmacology & pharmacy*, 2020, **11**, 12, 373-401.
22. Jelena Velebit Marković, Anemari Horvat, Tina Smolič, Sonja Prpar Mihevc, Boris Rogelj, Robert Zorec, Nina Vardjan, "Astrocytes with TDP-43 inclusions exhibit reduced noradrenergic cAMP and Ca^{2+} signaling and dysregulated cell metabolism", *Scientific reports*, 2020, **10**, 1, 6003.

Review Article

1. Tanja Jakoš, Anja Pišlar, Urša Pečar Fonović, Janko Kos, "Lysosomal peptidases in innate immune cells: implications for cancer immunity", *Cancer immunology and immunotherapy*, 2020, **69**, 2, 275-283.
2. Abida Zahirović, Jernej Luzar, Peter Molek, Nika Kruljec, Mojca Lunder, "Bee venom immunotherapy: current status and future directions", *Clinical reviews in allergy & immunology*, 2020, **58**, 326-341.
3. Mojca Lunder, Tomaž Bratkovič, Borut Štrukelj, "Supportive therapy for covid-19 and preventing SARS-CoV-2 infection", *Farmacevtski vestnik*, 2020, **71**, 2, 141-147.
4. Mojca Lunder, Anja Pišlar, Borut Štrukelj, Urša Pečar Fonović, Tomaž Bratkovič, " Modern pharmaceutical biology: traditional to innovative therapies", *Farmacevtski vestnik*, 2020, **71**, 1, 45-53.
5. Spase Stojanov, Aleš Berlec, "Electrospun nanofibers as carriers of microorganisms, stem cells, proteins, and nucleic acids in therapeutic and other applications", *Frontiers in bioengineering and biotechnology*, 2020, **8**, 130.
6. Tina Vida Plavec, Aleš Berlec, "Safety aspects of genetically modified lactic acid bacteria", *Microorganisms*, 2020, **8**, 2, 297.
7. Spase Stojanov, Aleš Berlec, Borut Štrukelj, "The influence of probiotics on the firmicutes/bacteroidetes ratio in the treatment of obesity and inflammatory bowel disease", *Microorganisms*, 2020, **8**, 11, 1715.
8. Tomaž Bratkovič, Janja Božič, Boris Rogelj, "Functional diversity of small nucleolar RNAs", *Nucleic acids research*, 2020, **48**, 4, 1627-1651.
9. Anja Pišlar, Ana Mitrović, Jerica Sabotič, Urša Pečar Fonović, Milica Perišić, Tanja Jakoš, Emanuela Senjor, Janko Kos, "The role of cysteine peptidases in coronavirus cell entry and replication: the therapeutic potential of cathepsin inhibitors", *PLOS pathogens*, 2020, **16**, 11, e1009013.

Short Article

1. Ana Koren, Mojca Lunder, Peter Molek, Peter Kopač, Abida Zahirović, Pia Gattinger, Irene Mittermann, Rudolf Valenta, Peter Korošec, "Fluorescent labeling of major honeybee allergens Api m 1 and Api m 2 with quantum dots and the development of a multiplex basophil activation test", *Allergy*, 2020, **75**, 7, 1753-1756.

Published Conference Contribution

1. Borut Štrukelj, "Novosti na področju razvoja cepiv proti SARS-CoV-2", In: *COVID-19: preventiva, diagnostika in terapija: strokovno izpopolnjevanje s področja farmacije*, Zbornik prispevkov, Univerza v Ljubljani, Fakulteta za farmacijo, 2020, 18-25.
2. Anja Klančnik, Katarina Šimunović, Dina Ramić, Meta Sterniša, Jerica Sabotič, Sonja Smole Možina, "Targeting *Campylobacter* adhesion in the fight against antimicrobial resistance", In: *Conference Food, Nutrition, Health*, Proceedings, Evropska mreža deklaracije za hrano, tehnologijo, prehrano za zdravje, 2020, 327-334.

Independent Component Part or a Chapter in a Monograph

1. Borut Štrukelj, "Resveratrol", In: *Minerali, vitamini in druge izbrane snovi*, Slovensko farmacevtsko društvo, 2020, 496-503.

Theses and Mentoring

1. Ana Bajc Česnik, *Impact of genes linked to amyotrophic lateral sclerosis on biochemical properties and cellular localization of the TDP-43 protein:* doctoral dissertation, Ljubljana, 2020 (mentor Boris Rogelj).
2. Tanja Jakoš, *The role of cathepsin X in antitumor immune response:* doctoral dissertation, Ljubljana, 2020 (mentor Janko Kos; co-mentor Anja Pišlar).
3. Abida Zahirović, *Identification and characterization of major bee venom allergen Api m 1 mimotopes for development of specific immunotherpy:* doctoral dissertation, Ljubljana, 2020 (mentor Mojca Lunder; co-mentor Peter Korošec).

DEPARTMENT OF ENVIRONMENTAL SCIENCES O-2

Head:
Prof. Milena Horvat

The Department of Environmental Sciences focuses on the interweaving of the physical, chemical and biological processes that shape our environment, humans and their activities. Our research is interdisciplinary and multidisciplinary, and takes place in several areas, such as Environmental analytical chemistry, Biogeochemical cycles, Microbial ecology, Environment and health, Environmental technologies, Risk and environmental assessment, and Environmental monitoring. We also work on the development of technical solutions for environmental problems and environmental management. The department hosts the "ISO-FOOD" ERA Chair for isotope techniques in food safety, quality and traceability, the infrastructure Centre of Mass Spectrometry (CMS) and the Mobile Ecological Laboratory Unit (ELME).

Analytical chemistry of the environment and biological systems

The role of chemical trace elements and their impact on the environment and living organisms depend not only on their total concentration, but also on the chemical forms in which they are present. Therefore, our research is focused on the development of new analytical procedures for the determination of elements and their chemical species (Al, Cr, Sn, As, Hg, Br, Pt, Ru, Ni, V, Zn) in environmental and biological samples.

In the field of ***elemental speciation***, the analytical performances of the low-pressure and high-pressure conjoint liquid chromatography (CLC) monolithic columns, assembling one convective interaction media (CIM) protein G and one weak anion-exchange diethylamino (DEAE) disks, which enable the two-dimensional separation in a single chromatographic run, were evaluated by comparing their robustness, selectivity, repeatability and reproducibility in the speciation of Pt-based chemoterapautics in human serum.

A novel, robust, rapid, sensitive and reliable analytical method based on monolithic chromatography (4 CIM DEAE disks, assembled into a column) coupled to UV and ICP-MS detectors was developed for ***Cr speciat***ion in human serum. Cr(VI) was separated from Cr-transferrin (Cr-Tf) and Cr-albumin (Cr-HSA). Good selectivity and method repeatability (RSDs below 8%) enabled an investigation of the kinetics of interaction of Cr(VI) and Cr(III) with serum constituents.

We offered analytical support to the Department for Nanostructured Materials in investigations of the recycling of rare-earth elements and transition metals from Nd-Fe-B magnets.

Within the framework of the SRA project Non-traditional isotopes as identifiers of authigenic carbonates we developed and optimised analytical methods for the determination of $\delta^{26/24}$**Mg** and $\delta^{88/86}$**Sr** in surface water and soil by MC-ICP-MS. The optimised procedures were tested on water and soil samples from the karstic aquifer of the Ljubljanica river and for the characterisation of bottled water in the Slovenian market. We optimised analytical methods for the determination of the isotopic composition of uranium in water and rock samples using multi-collector ICP mass spectrometry (MC-ICP-MS). Using $^{238}U/^{234}U$ activity ratios and δ^{238}U values in springs, in river water and in bedrock, and established the interdependencies of U isotope ratios and discharge, we were able to provide a better insight into the recharge, flow paths and mixing of ground- and surface-water in the karst aquifer of the Ljubljanica.

New methods for ***Sr isotope ratio*** determination in milk and olive-oil samples were developed and optimised using MC-ICP-MS. The optimised method was applied for the geographical discrimination of Slovenian milk.

In the field of ***organic analysis***, an analytical method for the determination of ***bisphenols*** (BP) in both the aqueous and algal biomass phases was developed. As part of the study of the cycling of ***CEC compounds*** (Contaminants of Emergent Concern), we developed a sensitive analytical method for the determination of selected estrogens, namely, 17-beta-estradiol (17βE2), 17-alpha-ethinylestradiol (17αEE2) and estrone (E1) in surface waters EMPIR Metrology for monitoring endocrine disruptors according to the Water Framework Directive). The results of the project will include validated reference methods based on mass spectrometry as a contribution to CEN / TC 230 and ISO / TC 147, reference materials and the implementation and evaluation of an interlaboratory comparative analysis for the determination of selected compounds in surface waters.

Dual detecting platforms for the ***adsorption of mercury (Hg) species*** were designed using crosslinked chemistries. Graphitic carbon nitride (g-C_3N_4) and sulfur-doped graphitic carbon nitride (*S*-g- C_3N_4) nanosheets were synthesized and characterized with a battery of techniques. The nano-impregnated sheets were successfully introduced in the 3-dimensional (3D) structure to facilitate a large surface area for the binding of Hg^0 and Hg^{2+}.

Figure 1: Calibration of mercury-emission measurements with traceable calibration methods developed in the MercOx project was used in field measurements at Salonit Anhovo (above) and at the thermal power plant in Marl, Germany (below)

Nanobuds and aerogels are promising with respect to the selective binding of Hg in laboratory-based settings. Further work on optimization and deployment are in the pipeline.

Metrology - the science of measurement is crucial for the department as most research is related to measurements or the use of measurement results. The department is a designated institute of the national metrology system for the amount of substance, particularly for trace elements in organic and inorganic materials.

We have developed metrological concepts for the determination of mercury and its compounds in air and flue gases within the European EMPIR (European Metrology Program for Innovation and Research) project MercOx (Traceability of oxidized mercury in air), coordinated by the department. The newly developed calibration system will significantly improve the comparability of results globally, which is crucial for the validation of models as a tool for decision makers. Based on the excellent results, the calibration procedures are now in the standardization phase, which is the subject of work within the new EMPIR Hg-SI project.

Metrology concepts have also been developed in additional areas of measurement science including traditional stable-isotope analysis of light elements covers: (i) development of new reference materials for environmental (greenhouse gases such as CO_2 and CH_4 as a part of EMPIR SIRS and STELLAR projects) and food (plant and animal origin) studies; (ii) evaluating the measurement uncertainties in these materials; and (iii) participating in the inter-laboratory comparisons at the highest metrology level (CCQM-K167). In the framework of the EMPIR SIRS project the evaluation of the expanded uncertainty of newly produced CO_2 reference materials with various isotopic compositions to cover the range of isotope ratios observed in the atmosphere was performed using EUROPA Scientific IRMS with the TG preparation system.

The department is also actively involved in two networks related to metrology: the ESFRI Infrastructure for promoting Metrology in Food and Nutrition (METROFOOD-RI) where JSI coordinates Slovenian Joint Research Unit and EMPIR FoodMetNet (Support for a European Metrology Network on Food safety) accepted in 2019.

As a Designated Institute (DI) for „Amount of Substance: Trace elements in inorganic and organic materials", we participated in the following studies in 2020:

- CCQM-K144 Trace elements in alumina powder (organized by KRISS from South Korea),
- CCQM-K145 Toxic and essential elements in bovine liver (organized by NIM from China),
- SIM.QM-S10 Trace elements in skimmed-milk powder (organized by NRC from Canada and INTI from Argentina),
- CCQM-K155 Elements and Tributyltin in Seawater (organized by GLHK from China and TUBITAK UME from Turkey),
- Participation in the characterization of new certified reference materials: ERM-CZ110 Fine dust (PM2,5-like) and IAEA-475 Marine Sediment prepared by JRC Geel (Belgium) and IAEA-MESL (Monaco).

Figure 2: CMCs – Calibration and Measurement Capabilities

Biogeochemistry and climate change

We started the EU MCSA ITN GMOS-Train project, which is the first project of its kind in Slovenia. It aims to provide much-needed education on mercury reduction at the global level within the UNEP Minamata Convention and specially to fill key gaps in the knowledge of **biogeochemical mercury cycling**, which links anthropogenic emissions and the accumulation of mercury in marine organisms.

Within the framework of the Trageted research programme (CRP), identification of **Pb sources** in the upper Mežiška valley based on Pb isotope composition, different Pb selective resins (Sr-resin, Pb-resin and Dowex 1-X8) for Pb isolation from water, plant, soil and sediment matrices were evaluated in terms of their efficiency of recovery and Pb isotope fractionation. The one with the best results will be subsequently used for the source identification of Pb in dust particles in the upper Mežiška valley.

We collaborated with researchers from Niš University (Serbia) in investigations of the toxicity of **cerium oxide nanoparticles** (CeO_2NPs) in non-biting midges. The results indicated that exposure to CeO_2NPs-contaminated freshwater sediments does not pose a risk to chironomids under environmentally relevant concentrations. However, the significant accumulation of CeO_2NPs by chironomid larvae may pose a risk through trophic transfer to organisms further up the food chain.

In collaboration with the Institute Nazionale di Oceanografia e Geofisica Sperimentale – OGS Trieste, Italy a mesocosmos experiment was performed in order to decode how different sources (natural, anthropogenic) of ***CO_2 influence biological systems*** (phytoplankton) using stable carbon isotopes. The experiments prove that phytoplankton isotopic composition quickly responds to changes in the $\delta^{13}C$ of the medium, making this approach a promising and low-impact tool for detecting CO_2 submarine leakages from carbon capture sites (CCSs).

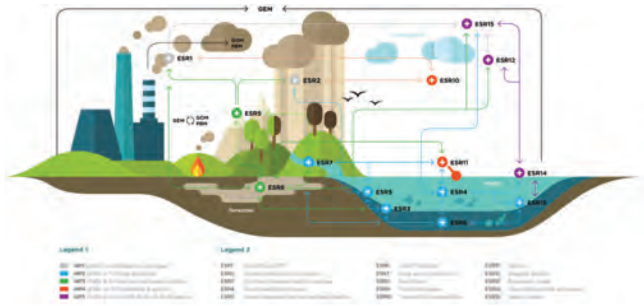

Figure 3: The structure of the MSCA ITN GMOS-Train project connects the work of 15 young researchers, doctoral students at 10 top research institutions in Europe.

In order to collect evidence of the possible occurrence of anaerobic oxidation of ***methane*** (AOM) at the sediment-water interface and infer the entity of the associated methane flux, the analyses of bulk sulphide minerals $\delta^{34}S$, total organic carbon and redox-sensitive elements were combined. The research was performed in the drift area of the Kveithola trough, a glacially-carved depression located in north-western Barents Sea, where active fluid escapes have recently been recognised. According to the negative values of $\delta^{34}S$ within the extracted solid sulphur phases (up to –49.1‰ for pyritic sulphur), organo-clastic sulphate reduction and/or disproportionation of sulphur intermediates result to be the only active processes in the near-surface sediments of the study area. However, moderate-to-strong enrichments of Mo detected in the relatively organic carbon-poor intervals of both the two cores suggests that the sulphidic conditions favouring Mo enrichments have been produced by AOM. Therefore, we can infer that the Kveithola trough experienced high methane fluxes that occasionally moved upwards in the sulphate-methane transition zone, inducing intense AOM in the proximity of its sediment-water interface.

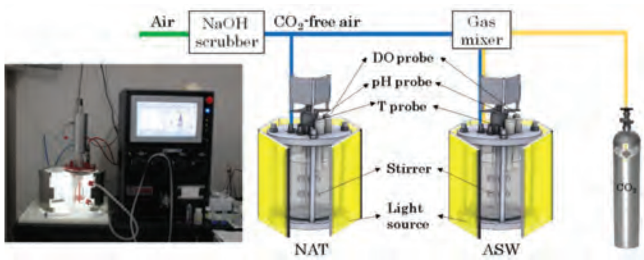

Figure 4: Schematic description of photobioreactors used for the three T. rotula culture experiments. NAT: natural seawater medium; ASW: artificial seawater medium. During algal growth, only CO_2-free air was used (on:off cycle: 10:50 min) in both media. Note that $CO_{2(g)}$ from a cylinder was only supplied during ASW medium preparation. Dissolved oxygen (DO; % sat), temperature (T, °C) and pHNBS were recorded by on-line probes. Light:dark regime: 14:10 h; continuous gentle stirring. Photobioreactor outline modified from Kbiotech®.

The post-fire effects on leaf development, leaf carbon isotope composition ($\delta^{13}C$), radial growth patterns and the xylem and phloem anatomy in undamaged (H-trees) and fire-damaged trees (F-trees) of Quercus pubescens Willd was investigated to better understand ***tree–fire–climate interactions*** for predicting the impact of the changing environment on tree functioning. It was found that the growth of leaves in F-trees relied more on the recent photosynthates than on reserves due to the fire disturbed starch accumulation in the previous season. A novel approach by including phloem anatomy in the analyses revealed that the fire caused changes in the conduit dimensions in the early phloem but not in the earlywood. However, the premature formation of the tyloses in the earlywood vessels of the youngest two xylem increments in F-trees implies that xylem hydraulic integrity was also affected by the heat.

The study performed in collaboration with ZRS-SAZU includes the evaluation of 6600 years of human and climate impacts on lake-catchment and vegetation in the Julian Alps (Lake Bohinj, Slovenia) using mineralogical, sedimentological, geochemical, stable isotope ratios of C and N, and pollen analysis. It was found that in the Bronze and especially the Iron Age (3500–2500 yr cal BP), when the region was, according to archaeological data, densely populated, clearing of forests due to agriculture, livestock production and metallurgical activities was detected through Cerealia type pollen, Plantago lanceolata, and the decline of Abies. In the subsequent centuries human impact on the environment continued (increased), but it seems that the watershed was not destabilised again. Several periods of high terrigenous input were recorded at 6100–6000, 5700–5550, 5000–4600, 3900, 3700–3550, 2300–2200 yr cal BP and could be associated with a mobilisation of river inflow from the eastern flysch bearing catchment, due to river migration during periods of a wetter climate. These flood patterns match with periods of enhanced flood activity in the wider Alpine region. The results were published in the paper Quaternary Science Review, which was selected by the Slovenian Research Agency as the outstanding scientific achievement in the field of Archaeology and Geology in 2020.

Analysis of the organic residues and experimental archaeology enabled us to characterise the ***fuel source and wick remains*** of two prehistoric lamps from Zgornje Radvanje (NE Slovenia) from the Copper Age settlement. Identification and stable isotope composition of lipids absorbed in the artefacts indicate the predominant use of ruminant fat as a fuel burned for illumination, possibly in combination with plant oils.

In collaboration with the Atomic Centre of Bariloche, Argentina, we explored the geochemical and mineralogical characteristics of sediments in Lake Futalaufquen, exposed to the volcanic ejecta of Andean volcanism in Northern

Patagonia and evaluated their potential as ***paleoclimate proxies***. We also participated in a multinational study of controls that affect the structure and timing of deglaciations with a focus on Termination II (the penultimate deglaciation). Based on a detailed study of sedimentological, palinological and isotopic characteristics a tufa formation in Trabaque (Iberian Peninsula), we were able to describe a sequence of events and the mechanisms that controlled the structure and timing of the complete T-II by integrating the evidence from the Nordic Seas and the North Atlantic, along with their influence in the Mediterranean region, and the response of the Southern Hemisphere.

In collaboration with the National Institute of Biology, we participated in a study of the colonization of microorganisms from activated sludge on different types of ***plastics*** and the potential degradation of substrates. It was found that sludge bacteria can thrive on commonly used plastics (PET, HDPE), and that the diversity and community structure in the biofilm depends upon the chemical composition and surface characteristics of the plastic substrate.

Water cycle

We have investigated the behaviour of ***uranium isotopic ratios*** in the karstic rivers Krka in Slovenia and Croatia. It was found that uranium isotopic differences reflect the changing bedrock lithology and the mixing of waters from different sources. Fractured carbonate rocks weather more rapidly, with higher removal of ^{234}U from rock to water due to the alpha recoil effect and higher $^{234}U/^{238}U$ activity ratios. Less-permeable and less-soluble rocks allow less oxidation of U(VI), while the alpha recoil effect cannot play such a significant role, which results in a lower $^{234}U/^{238}U$ activity ratio. Isotopically lighter uranium co-precipitates preferentially with carbonate in flowstone and tufa without fractionation. Therefore, uranium isotope ratios in terrestrial carbonate formations reflect both the storage of CO_2 and the amount uranium bond to detrital material.

In collaboration with colleagues from the Hungarian Academy of Science and Arts, the Isoscape – a time series of distribution maps of amount-weighted ***annual mean precipitation tritium*** in Adriatic-Pannonian region in 1976 to 2017 – was published in Earth System Science Data after 40 years of systematic analyses of isotope composition of precipitation. A part of this long-term effort is also the SLONIP – Slovenian Network of Isotopes in Precipitation, which enables on-line public access to oxygen and hydrogen isotope data in precipitation in Slovenia and was first published in 2020 (https://slonip.ijs.si/).

In collaboration with the Public Utility of Podgorica (Montenegro) we conducted the first isotope study of the Mareza karst aquifer, which is the main drinking water source for the capital of Montenegro. Based on the isotopic composition of water in precipitation, in the Zeta river and in main springs of Mareza, we estimated the ***origin of groundwater***, the mean altitude of the recharge area and proved that there is no notable communication between the Zeta river and the springs.

Using isotopic tools ($\delta^{18}O$, $\delta^{2}H$, $\delta^{13}C_{DIC}$, $^{87}Sr/^{86}Sr$) and the element of the footprint, we characterized Slovenian bottled mineral water and described the basic geochemical characteristics of their springs.

Atmosphere research

Diurnal and synoptic variations of radon activity concentrations have been combined for the first time applying the radon-based classification techniques of air mixing to better understand air-quality variability in the sub-Alpine Ljubljana Basin. Using hourly averages of values of meteorological parameters (wind speed, changes of air temperature, solar radiation, precipitation), air-quality parameters (NO_2, CO, PM_{10}, BC-black carbon, SO_2, O_3) concentration and radon (^{222}Rn) activity concentration during two consecutive winters. In total, six air-mixing classes have been defined for each winter: five diurnal and one synoptic (persistent temperature inversion – PTI, which has been internally separated as "strong" or "weak"). Diurnal and synoptic changes in a mixing state have appeared to play an important role in air-quality variability in both winters. For mixing classes #1 to #3 (wind speeds ≥1.5 m s^{-1}), a small diurnal accumulation of local pollutants (CO, NO_2, PM_{10} and BC), but significant remote contributions to SO_2 and O_3 concentration have been observed. During the class #5 and PTI days (the most stable conditions, characterised by the nocturnal wind speed of ≤0.5 m s^{-1} or rates of air temperature change at 2 m of ≥1.5 °C h^{-1}), have been associated with the worst air-quality conditions. The research was performed within the STRAP project (Sources, transport and fate of persistent air pollutants in the environment of Slovenia).

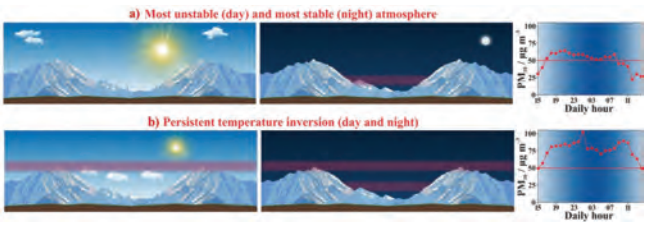

Figure 5: Atmospheric mixing conditions over the basin terrain and diurnal composite plots of particulate matter (PM10) concentration: a) during the atmospheric most unstable day and most stable night, and b) during the atmospheric persistent temperature inversion during day and night

In determining highly time-resolved and source-separated black carbon emission rates, a study conducted by the Aerosol company, our hourly averages of atmospheric radon activity concentration in Ljubljana and in Ajdovščina (Vipava Valley) were used to determine the mixing-layer height for periods of thermally driven planetary boundary layer evolution.

Coloid biology

In 2020, research was carried out under two European projects: UIA funded "Applause" project (Alien Plant Species - from harmful to useful with citizens' ice activities) and EU-H2020 funded "GREENER" project (InteGRated Systems for Effective ENvironmEntal Remediation), where we used the previously developed methods for combining cells into ***artificial multi-cellular structures***, i.e., aggregates and biofilms, where bacterial cells are glued together with particles or on different types of surfaces. We constructed 2D and 3D structures of different composition size and thickness. A patent of this innovative approach has been submitted and moreover, based on these methods, we were able to show *in vitro* the importance of the proximity between two cells to exchange nutrients between each other. The characteristics of nutrient exchange between bacterial cells, which was theoretically modeled was thus practically proven.

By combining different bacteria in such structures, metabolic coupling can be performed for different applicative solutions. As part of the mentioned project we have investigated the ***transformation of lignin to vanillin*** and cellulose into polyhydroxyalkanoates and the degradation of polycyclic aromatic hydrocarbon pollutants. Using the electrostatic aggregation of particles and fibres we have developed materials alternative to paper using waste plant biomass and waste polyelectrolytes like chitosane.

As part of the national project ARRS N1-0100 we carried out several experiments to construct ***artificial biofilms*** on surfaces that will be exposed in sea water. The work has already been submitted to the journal Frontiers in Materials.

Together with the group for radiochemistry we started a national project (ARRS J7-2597) for selective ***enrichment of tritium*** using microbes. We have started to prepare the methodology and microbial strains to be used in the preliminary experiments.

In two other national projects (ARRS J1-9194, ARRS J3-1762), we have been collecting and characterizing bacterial isolates from the oral cavity and the skin surface of babies. We prepared the methodology of ***genome sequencing*** and annotation to be implemented for the selected isolates.

In the CROSSING project (collaboration between JSI and HZDR, Germany), we analysed the interactions between bacteria and nanoparticles and bacteria and metal surfaces with different physical characteristics obtained by nano printing and etching.

In collaboration with the Chemical Institute, as part of a post-doc project, we prepared a system for the purification of different organic pollutants used in paper making, which was based on a bacterial immobilization system and hve demonstrated the proof-of-concept for such a purification system.

In the framework of international cooperation, we started a new project ***"SurfBio"*** funded by EU-H2020, which will help introduce the field of colloid biology and strengthen research activities at the Jožef Stefan Institute. In relation to the JSI Post Graduate School new curricula will be introduced to produce new interdisciplinary PhD theses.

Environment and health

In the field of national and European humane monitoring, we continued to recruit children and adolescents in the wider area of Slovenia. Exposure of children and adolescents to the herbicides glyphosate and AMPA living in rural areas of northeastern Slovenia is very low. We have shown that the Slovenian population is exposed to various mobile organic compounds such as bisphenols and phthalate compounds through food and the use of products, which are present in plastic packaging, cans, personal care products, PVC); lifestyle and habits also affect exposure to phthalates (e.g., living space, time spent outside). Parabens are primarily associated with the use of makeup. The studies report exposure of children and adolescents in Slovenia to a wide range of different endocrine-disrupting chemicals for the first time, connecting it to exposure patterns and exposure sources, and investigates the direct connection between levels of urinary endocrine-disrupting chemical biomarkers and genetic polymorphism in UGT2B15. Moreover, the exposure of mothers and their children to organophosphate and pyrethroid pesticides has also been assessed for the first time. We also studied the protective role of selenium in association with APOE ε4 in early life.

In the context of European human biomonitoring (HBM4EU), we focused in particular on the topic of ***cadmium exposure in Europe***. We want to answer the question of what proportion of cadmium exposure is represented by contaminated soils. For this purpose, we combined HBM data and geospatial data were collected from available European databases (Cd concentration in the topsoil FOREGS and LUCAS geochemical databases; percentage of arable land; consumption of inorganic fertilizers; agricultural areas; total and land area; motorway density and other roads). In addition, the JSI prepared a document on ***arsenic compounds*** in the environment, human exposure, possible and recorded health effects, health-risk assessment and related practices. The department was also involved in the preparation of documents for the continuation of HBM4EU in the framework of the PARC (Horizon Europe) project, which aims to develop an integrated approach to risk assessment in relation to chemicals in the human environment. We have also participated in the second, third and fourth Interlaboratory Comparison Investigations (ICI) on Cr in whole blood, serum and urine.

In the framework of the NEURODYS project, we have continued recruitment of pregnant women in the Celje region, with an aim to study the effects of various environmental factors on exposure to environmental chemicals and the development of children following the "***exposome***" approach. This cohort study will provide valuable biological samples to perform not only chemical and basic molecular analysis, but also analysis of metabolome, epigenome, transcriptome, and microbiome. In order to approach the complete exposure assessment, we have performed some additional chemical and molecular analyses in the existing birth cohort PHIME-CROME. Results have been combined with the existing ones and a joint database has been established, which now includes: prenatal exposure to trace elements, exposure to trace elements and organophosphorous pesticides at 7–8 years of age, neuropsychological scores at 18 months and 7–8 years of age, biomarkers of genetic susceptibility, and accompanying data such as life-style and home-environment data. The methodology to study the influence of microbiome on exposure as well as development has been established and validated. In order to study associations between environmental parameters, genetic predisposition, and neuropsychological development, we have used classic statistical approaches as well as machine-learning methods. Preliminary results are already available, the overall findings will be published in 2021.

The possibility to use stable ***carbon isotopes of fatty acids*** ($\delta^{13}C_{FA}$) in human milk as a biomarker of different food consumption was investigated, since all of the carbon in our bodies derives from the food we eat. The research performed on 74 mature human milk from two contrasting Slovenian areas (coastal and inland) indicated that this approach significantly improves the information on seafood consumption.

Having recognised the extremely important role of compound annotation in exposome characterisation, we studied the basic principles of the cutting-edge ***cheminformatics mass-spectrometry-based*** approaches employed in the exposome annotation. In this view we defined the three crucial cheminformatics tasks, including molecular formula assignment, compound prioritization and compound annotation. We assessed the performance of different approaches through the ability to annotate exposome constituents.

While being involved in a ***pharmacokinetic study*** of an opioid drug fentanyl, we witnessed an accidental intoxication of a pig after ingestion of a fentanyl transdermal patch. We were able to associate the intoxication with the highly elevated levels of fentanyl in the pig's blood.

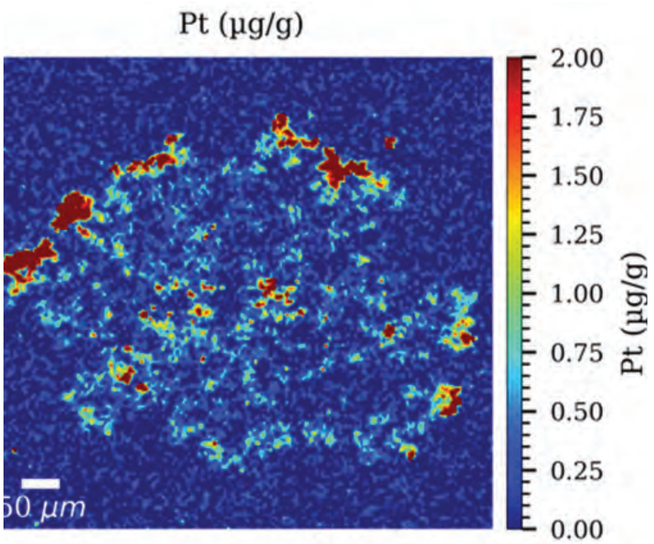

Figure 6: Quantification of Pt in a cisplatin-treated tumor spheroid by the LA-ICP-MS isotope dilution method

In the field of ***metal bioimaging***, we optimized laser ablation (LA) parameters to quantify the ablated sample by ICP-MS. We are currently developing several analytical methods for the biological bio-visualization of various samples (tissues, tumor spheroids, and cells) using matrix standards and the isotope dilution (ID) technique for quantification. So far, ID has proven to be the most accurate method of quantification, as it also serves as an internal standard for instrument drift correction. An example of the successful quantification with the LA Pt visualization technique in cisplatin-treated tumor spheroids is shown in Figure 6.

In the field of ***wastewater-based epidemiology*** (WWE) numerous studies have been published relating to the back-calculation of drug consumption based on the analysis of wastewater influents from municipal wastewater treatment plants. Less commonly, WBE is used for site-specific studies. Accordingly, we prepared a review article on published WBE-based studies on drug-use trends in educational institutions and prisons, and at music festivals, sporting events, and holidays. In the article, we presented a discussion on the use and benefits of using WBE in these specific cases and an overview of current challenges and future perspectives. In addition, wastewater analysis investigates the prevalence of drugs in Slovenian educational institutions according to the level of education offered (primary, secondary and higher education), geographical location (comparison between municipalities) and the degree of urbanization (urban vs. non-urban areas). The processing of the results is still ongoing. Based on the conclusions so far, we confirm that the analysis of wastewater provides a non-invasive insight into the trends of drug use in educational institutions.

Food/nutrition

The isotopic ratio ***^{87}Sr / ^{86}Sr*** was determined in milk, feed and water samples from Italy. Thus, we wanted to examine which factor (feed or water) has a greater influence on the isotopic composition of Sr in milk. In this way, the ^{87}Sr / ^{86}Sr ratio in milk could be linked to the environment and this information could be used to verify the geographical origin of the milk. The ^{87}Sr / ^{86}Sr ratio was also used for honey from Montenegro and argan seeds from Morocco for the purpose of determining the geographical origin.

In food-related studies, we developed an analytical method for the determination of ***neonicotinoids*** in propolis and applied it to a series of commercially available products. The optimised method was applied to 30 samples: 18 raw propolis and 12 ethanol tinctures. Acetamiprid, imidacloprid, and thiacloprid were detectable in seven samples, but were still below the LOQ. We concluded that only low contamination with selected neonicotinoids was present in real samples. This study is the first to report the determination of several neonicotinoid residues in propolis.

We also studied the migration of twelve ***bisphenols*** (BPs) from beverage cans and reusable steel and plastic sports bottles using a validated GC-MS/MS method with ng L^{-1} LOQ. This work demonstrates that among BPs, BPA remains the primary bisphenol in FCMs, but at the same time confirms the presence of other BPs in FCMs. It is also clear that the leaching of bisphenols is conditioned by the food/drinks stored in FCM containers, which has been shown with different simulants. Importantly, we show that consuming beverages from cans is more concerning than consuming beverages from reusable sports bottles. Our findings provide insights into the problems surrounding the migration of chemicals from FCM and lower the risk to consumer health. Currently, non-target workflows have been developed to elucidate FCM leaching to food/beverages.

The presence of various ***inorganic nanoparticles*** was determined in selected food products using an optimized single-particle ICP-MS technique. The highest concentrations of nanoparticles (in the range of mg/g) were found in food samples that contained additives or food additives (such as E 172, E 551, E 171). The same analytical technique was also used to determine the presence of iron oxide nanoparticles in E 172 food pigments and to characterize titanium dioxide (E 171) food additives in confectionery products as part of an inter-laboratory comparison.

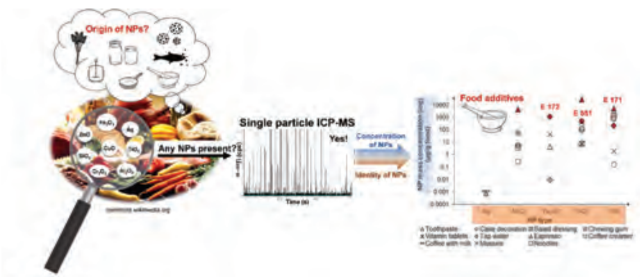

Figure 7: Using the single-particle ICP-MS technique, we determined the presence, type, and concentration of inorganic nanoparticles in different food samples.

In the framework of the ***ERA Chair ISO-FOOD*** the protocol for determination of the authenticity and traceability of different food was established. This includes: (i) development of standard operational procedures and optimization of the methods using a response surface methodology (RSM) and artificial neural network (ANN); (ii) database creation and visualization of the data; (iii) modelling using multivariate statistical methods such as Linear Discriminant Analysis (LDA), Orthogonal Partial Least Squares Discriminant Analysis (OPLS-DA) and Data Driven - Soft Independent Modelling of Class Analogy (DD SIMCA); and (iv) discrimination according to the species, cultivars, types, geographical origin and agricultural practice.

The approach was applied to different food commodities including milk and dairy products, garlic, chicory plants (*Cichorium intybus L.*), truffles and argan oil. The obtained data on milk, truffles and argan oil are also included in the e-component of different EU projects such as METROFOOD-RI research infrastructure, REALMed and FNS-Cloud. In 2020 the expert task of checking the origin of fruits and vegetables was performed for the Administration of the Republic of Slovenia for Food Safety, Veterinary and Plant Protection including strawberries, cherries, apples, kaki, asparagus and garlic. Statistical models indicated that on average 37% of the samples are unlikely to originate from Slovenia.

Environmental technologies

We continued research on ***cement-organics-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 conducted initial irradiation of three types of superplasticizers and identified changes in the FTIR spectrum in samples caused by gamma radiation. The work is on-going with identification of the degradation products.

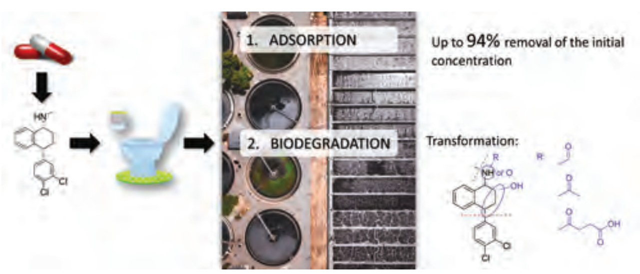

Figure 8: Sertraline, an antidepressant, is removed from wastewater by adsorption. Its biodegradation is affected by the presence of rapidly biodegradable carbon. Despite the high removal efficiency, sertraline is still reported in the environment. Seven new biotransformation products have been identified. The identified biotransformation products are present in wastewater.

We have started to develop a new, innovative technology for the ***bio-based separation of tritium*** from water within the ARRS BIOTRISEP project. Cyanobacteria, algae and sulphate reducers are planned to be investigated and exploited for this purpose.

Our research related to environment cycling and wastewater treatment has continued to address industrial chemicals, including BPA and its alternatives. Our focus has been on ***advanced wastewater treatment***: biological (algal ponds) and abiotic (UV, photocatalytic, cavitation, novel coagulation with natural coagulant isolated from beans) treatment.

High-rate algal ponds (HRAP) are an alternative to conventional wastewater treatment that could contribute to the circular economy by valorising reclaimed water and algal biomass.

In collaboration with the Faculty of Chemistry and Chemical Technology (UL), we are currently studying the development of photocatalytic materials and composites as an inert support for treating wastewater. Their efficiency is being tested with a mixture of bisphenols having different physicochemical parameters.

With the collaboration of the University of Novi Sad, Serbia, we also investigated advanced ***non-oxidative treatments*** to remove CECs. A structure-property relationship (SPR) study revealed correlations between the removal efficiency of most treatments applied and the total polar surface area (TPSA) of the micropollutants.

A ***non-target screening approach*** was used to investigate the biodegradation transformation products of two ***bisphenols***, e.g., BPF and BPS, during biological wastewater treatment with activated sludge. For target analysis, GC-MS/MS was applied, while for the identification of biotransformation products (BTPs), we used LC-QTOF-MS. The results obtained in collaboration with the University of Antwerp, Belgium, revealed that BPF and BPS degrade readily and are unlikely to accumulate in biosolids or wastewater effluent. The first-order kinetic model revealed that BPF degraded faster than BPS and that the degradation rate decreases with an increasing initial concentration. The machine-learning algorithm adopted as part of the non-targeted workflow identified three known BTPs and one novel BTP of BPF, and one known and ten new BTPs of BPS. The data supports possible new biodegradation pathways, i.e., sulphation, methylation, cleavage and the coupling of smaller bisphenol moieties.

We continued to study the fate of CEC during WW treatment and in the environment. To mimic the ongoing processes during WW treatment, we performed different laboratory-scale experiments, including batch biodegradation and sorption experiments, and flow-through laboratory-scale pilot wastewater treatment bioreactors. These simulations were used to follow the fate of an antidepressant sertraline, where it was found that sorption to activated sludge was the leading removal process, and biodegradation was the secondary removal process (Figure7).

Under the same framework we also investigated the potential of ***molecularly imprinted polymers*** to serve as sorbents for the removal of CEC in WW treatment. The molecularly imprinted polymers demonstrated superior sorption capabilities in wastewaters and improved recycling properties as compared to the classic sorbent, granulated activated carbon.

To study the photochemical fate of the same group of compounds, i.e., ***antidepressants***, we performed photodegradation experiments in the presence of photosensitizers or reaction quenchers. Following the determination of rate constants, we were able to predict sertraline phototransformation kinetics by "Aqueous Photochemistry of Environmentally occurring Xenobiotics" (APEX) software. The results of the modelling were validated by irradiating the sertraline-spiked surface water by sunlight. The half-life, the predominant photodegradation processes and transformation products were determined on the lab scale and again, they were shown in Slovenian surface waters.

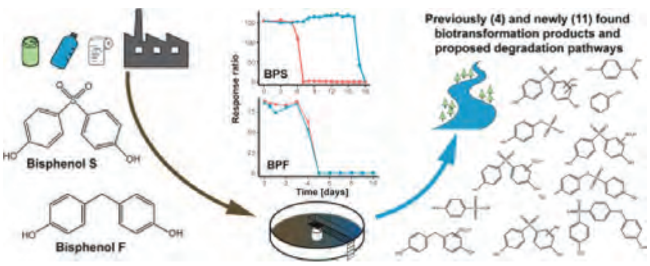

Figure 9: Kinetics and biotransformation products of bisphenol F and S during aerobic degradation with activated sludge

In parallel to the analytical evaluation of treatment processes, we have also examined the ***toxicity*** of BPA, BPF and their binary mixture towards primary producers, the eukaryotic green alga *Pseudokirchneriella subcapitata* and the prokaryotic cyanobacterium *Synechococcus leopoliensis*. The results demonstrated that *S. leopoliensis* is more sensitive than *P. subcapitata*, whereas the toxic potential of the two BPs is comparable and represents a comparable hazard for phytoplankton (Figure 4). The toxicity of the binary mixture was predicted by different models and compared to experimental data. The environmental risk characterisation based on comparing reported concentrations of BPA and BPF in surface waters to the predicted no-effect concentration values obtained in this study showed that BPA represents an environmental risk in some instances, whereas BPF does not. However, more data on the toxicity to aquatic species, including combined effect, and data on their occurrence in the aquatic environment are needed to enable environmental risk assessment of BP analogues.

Environmental management, environmental impact assessment and risk assessment

In 2020 we began the activities within the TransCPEarlyWarning project, which aims to improve the level of coherence of 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, homogeneity through the integration of existing early warning approaches and thus improving the exchange of information within the European Civil Protection Mechanism.

Within the HERA project (Health and Environment Research Agenda for Europe - Integrating Environment and Health Research: a Vision for the EU) we have been engaged in the identification of the research and policy needs, gaps and priorities on environment and health (co-organisation of workshop with stakeholders from Central

Europe); the work has also been oriented towards the research of the harmonised methodology in health impact assessment studies considering environmental factors and the societal and economic impacts thereof.

Novel approaches in environmental monitoring were tested using novel Earth Observation (EO) systems. To this end, we have continued the activities of using advantages of recent technological developments of sensor technologies, which aim at providing information on individual's exposure to environmental stressors, such as air and water pollution; using combination of in-situ and remote sensing, including participatory sensing approaches and modelling, and which also contribute to the Smart Cities concepts and building of Citizens Observatories. Work focused on characterization of an individual's living environment, with the emphasis on urban settings, using novel sensing technologies in combination with external sources of information supported by GIS tools and modelling, and the development of tools and methodologies for data aggregation and fusion to support integrated assessment of environmental pressures. To this end, we participated in the following EU funded projects that to a large extent are using various citizen science and community-based environmental monitoring approaches to gather relevant information: (i) ICARUS H2020 project dealing with the development of tools and strategies for urban impact assessment in support of air quality and climate change governance, and where volunteers participated in a sampling campaign using low-cost sensors for monitoring AQ and physical activity in their living environment; (ii) SMURBS ERA-Planet project promoting smart-city concepts and enhancing urban resilience to various urban pressures by integrating multiple Earth Observation (EO) sources information and decision making tools for individuals and communities; and (iii) CitieS-Health H2020 project where citizens are actively engaged in the co-design and conduction of experiments to explore how do the quality of the living environment and living habits affect the (mental) health and well-being of individuals.

We also successfully completed the SciShops.eu project (Improving the responsible and sustainable expansion of the network of scientific stores in Europe), within which we successfully partnered with the NGO Greenpeace Slovenia in analysing the carbon footprint of disposable plastic bottles and grave candles through the Center for Participatory Research at JSI.

A decision analysis for the waste disposal site Boršt at uranium mine Žirovski vrh has been made within MODARIA II programme (Modelling and Data for Radiological Impact Assessments), coordinated by the IAEA. We also contributed to the report of the MODARIA II Working Group 1 activities.

Environmental monitoring

In cooperation with the Environmental Agency of the Republic of Slovenia (ARSO), we performed control measurements of organotin compounds. We also monitored mercury in precipitation and elemental mercury in the air at the Iskrba reference station. In cooperation with the Croatian Water Environmental Agency, we continued measurements of organotin compounds and polybrominated diphenyl ethers in sea and river waters in 2020.

The monitoring of natural radionuclides within the influential area of the former uranium mine and mill at Žirovski vrh was performed. We also participated in off-site monitoring of Krško Nuclear Power Plant (NPP) with determination of strontium and tritium in environmental samples, as well as tritium and radiocarbon in gas effluents from the NPP. With analyses of strontium and tritium, we also participated in the monitoring of radioactivity in drinking water in Slovenia, as well as in the monitoring of the living environment in Slovenia. Methods used for the determination of strontium, tritium and radiocarbon for the monitoring purposes are accredited by the Slovenian accreditation body (SA LP-090).

Within the infrastructure RI-SI-EPOS project, we obtained in 2020 several modern instruments for monitoring radon and radon progeny activity concentrations in different environments.

The accreditation of radon measurements, in which our department, the Department of Low and Medium Energy Physics and the Radiation Protection Unit participate, was in 2020 extended to radon progeny.

Education

We have started a new EU H2020 project A-CINCH where the main focus is in development of virtual reality laboratory for radiochemistry education. For this purpose, we have developed scenarios for different exercises to be implemented into virtual laboratory. In collaboration with JSI Centre for Knowledge Transfer in Information Technology we started to expand educational videos for teaching of basics of analytical radiochemistry.

Infrastructural Centre for Mass Spectrometry (CMS)

CMS connects various mass spectrometers with which we conduct research and chemical analyses in research programmes and projects in the field of environmental pollutants, food and feed control and authenticity, the effects of various substances and chemicals on health, etc. CMS activity is carried out in the research areas of 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 protection. In collaboration with the other infrastructural centers in the field of structure and properties of substances, the CMS determines qualitative and quantitative analyzes 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, in the air, soil, soils, sediments, and similar.

Despite the limited scope of the 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

Within the Department of Environmental Science we also operate a mobile chemical laboratory of Ecological Laboratory with a Mobile Unit (ELMU), which is organised in the Civil Protection and Rescue System in Slovenia for intervention in the ecological accidents with hazardous substances and materials. The ELMU chemical mobile laboratory intervened eleven times in the field in 2020 due to environmental pollution, especially air pollution during fires or in in residential areas, spills of hazardous substances into the water streams and indirectly threatened sources of drinking water and because of irregular waste disposal. In addition to emergency response activities, members of the ELME mobile chemistry laboratory unit, trained their competence in regular ELME exercises, tested new equipment and improved the knowledge, procedures and analytical methods of the mobile ecological laboratory for the determination of hazardous substances in the environment. For this purpose, the unit was last year equipped with a portable Raman spectrometer.

Some outstanding achievements in the past year

1. Connection between levels of urinary endocrine-disrupting chemical biomarkers in human population and genetic polymorphism was demonstrated for the first time.
2. Development of a classification of atmospheric mixing in the basin based on variations in daily and synoptic radon concentrations
3. Software development for authenticity and traceability of food (www.foodtrack.ijs.si)
4. Development of a method for detection of the illegal watering of milk using $\delta^{18}O_{lactose}$ values as an internal standard
5. Development of a regional model (AP^{3}H) and maps of spatial and temporal of distribution of tritium activity concentration in precipitation in Adriatic – Pannonian region in 1976 to 2017.
6. New insights into the kinetics and biodegradation of bisphenols F and S during aerobic degradation by activated sludge.
7. Coordination of the EU MCSA ITN project GMOS-Train and Twining project SurfBio

Some outstanding publications in the past year

1. Andrič, Maja, Sabatier, Pierre, Rapuc, William, Ogrinc, Nives, Dolenec, Matej, Arnaud, Fabien, Grafenstein, Ulrich von, Šmuc, Andrej. 6600 years of human and climate impacts on lake-catchment and vegetation in the Julian Alps (Lake Bohinj, Slovenia). *Quaternary science reviews*, 2020, 227, 1-18. DOI: 10.1016/j.quascirev.2019.106043
2. Bergant Matic, Ščančar Janez, Milačič Radmila. Kinetics of interaction of Cr(VI) and Cr(III) with serum constituents and detection of Cr species in human serum at physiological concentration levels. *Talanta,* 2020, 218, 121199-1-121199-8, doi: 10.1016/j.talanta.2020.121199.
3. Kikaj, Dafina, Chambers, Scott D., Kobal, Matjaž, Crawford, Jagoda, Vaupotič, Janja. Characterizing atmospheric controls on winter urban pollution in a topographic basin setting using Radon-222. *Atmospheric Research*, 2020, 237, 1104838-1-1104838-12, doi: 10.1016/j.atmosres.2019.104838.
4. Kocman, David, Števanec, Tjaša, Novak, Rok, Kranjec, Natalija. Citizen science as part of the primary school curriculum : a case study of a technical day on the topic of noise and health. *Sustainability*. 2020, 12, 23, 10213-1-10213-15. DOI: 10.3390/su122310213.
5. Milačič Radmila, Ščančar Janez. Cr speciation in foodstuffs, biological and environmental samples: methodological approaches and analytical challenges: a critical review. TrAC, *Trends in Analytical Chemistry*, 2020, 127, 115888-1-115888-24, doi: 10.1016/j.trac.2020.115888.

6. Novak, Rok, Kocman, David, Robinson, Johanna A., Kanduč, Tjaša, Sarigiannis, Dimosthenis, Horvat, Milena. Comparing airborne particulate matter intake dose assessment models using low-cost portable sensor data. *Sensors*. 2020, 20, 5, 1406-1-1406-16. DOI: 10.3390/s20051406.
7. Potočnik, Doris, Nečemer, Marijan, Perišić, Igor, Jagodic Hudobivnik, Marta, Mazej, Darja, Camin, Federica, Eftimov, Tome, Strojnik, Lidija, Ogrinc, Nives. Geographical verification of Slovenian milk using stable isotope ratio, multi-element and multivariate modelling approaches. *Food chemistry*, 2020, 326, 126958-1-126958-11. DOI: 10.1016/j.foodchem.2020.126958.
8. Rovan, Leja, Lojen, Sonja, Zuliani, Tea, Kanduč, Tjaša, Petrič, Metka, Horvat, Barbara, Rusjan, Simon, Štrok, Marko. Comparison of uranium isotopes and classical geochemical tracers in Karst aquifer of Ljubljanica River catchment (Slovenia). *Water,* 2020, 12, 7, 2064-1-2064-29, doi: 10.3390/w12072064.
9. Runkel, Agneta, Snoj Tratnik, Janja, Mazej, Darja, Horvat, Milena. Urinary phthalate concentrations in the slovenian population : an attempt to exposure assessment of family units. *Environmental research : multidisciplinary journal of environmental sciences, ecology, and public health*. 2020, 186, 109548-1-109548-13. DOI: 10.1016/j.envres.2020.109548
10. Stajnko, Anja, Snoj Tratnik, Janja, Kosjek, Tina, Mazej, Darja, Jagodic Hudobivnik, Marta, Eržen, Ivan, Horvat, Milena. Seasonal glyphosate and AMPA levels in urine of children and adolescents living in rural regions of Northeastern Slovenia. *Environment international*. 2020, 143, 105985-1-105985-15. DOI: 10.1016/j.envint.2020.105985
11. Strojnik, Lidija, Camin, Federica, Ogrinc, Nives. Compound-specific carbon and hydrogen isotope analysis of volatile organic compounds using headspace solid-phase microextraction. *Talanta*, 2020, 16, DOI: 10.1016/j.talanta.2020.121264
12. Domínguez-Villar, D., Vázquez-Navarro, J. A., Krklec, K., Lojen, S., López-Sáez, J.A., Dorado-Valiño, M., Fairchild, I.J. Millennial climate oscillations controlled the structure and evolution of Termination II. Scientific reports. 2020, 10, 14912-1-14912-10. ISSN 2045-2322. DOI: 10.1038/s41598-020-72121-4.
13. Kern, Z., Vreča, P., Kanduč, T., Štrok, M., et al. Isoscape of amount-weighted annual mean precipitation tritium (^{3}H) activity from 1976 to 2017 for the Adriatic-Pannonian region - AP^{3}H_v1 database. Earth System Science Data 2020, 12(3), 2061-2073. ISSN 1866-3508. DOI: 10.5194/essd-12-2061-2020.

Awards and Appointments

1. Jan Kejžar: Krka's recognition for the master's thesis: Comparison of dietary supplements from algae: antioxidant potential and isotopic composition
2. dr. Aleš Lapanje: Slovenian Research Agency - EXCELLENT IN SCIENCE 2020: The most visible research achievements inspiring young generations. Area: Biotechnology. Title: How we made a live protective coating.
3. Nina Šiškovič: Biotechnical Faculty's Prešeren Award for 2020: Determination of volatile organic compounds in truffles
4. Žiga Tkalec: Best Poster Award on Exposome Symposium, New York, USA, Mount Sinai Institute for Exposomic Research, Development of an analytical method for nontargeted screening for organic contaminants in human urine.
5. Janja Vidmar: Jožef Stefan Golden Emblem Prize, Ljubljana, Jožef Stefan Golden Emblem Committee, PhD dissertation: "Quantification and sizing of metal-based nanoparticles in the environmental and biological samples"

Organization of conferences, congresses and meetings

1. Co-organization of the Ceremonial Annual Meeting of the Slovenian Association of Geodesy and Geophysics on the Occasion of the 25th Anniversary of the Admission of Slovenian National Committee of IUGG to the International Union of Geodesy and Geophysics (IUGG), Faculty of Civil and Geodetic Engineering, Ljubljana, 30 January 2020
2. Co-organization of the annual meeting of the Slovenian Association of Geodesy and Geophysics "Research in the field of geodesy and geophysics - 2019", Faculty of Civil Engineering and Geodesy, Ljubljana, 30 January 2020
3. Meeting within the MercOx project, Reactor centre JSI, Ljubljana, 2 March 2020
4. Meeting within the ICARUS project, Reactor centre JSI, Ljubljana, 9 March 2020
5. Co-organization of the HERA Regional Workshop - Central and Eastern Europe, 5 November 2020 (online)

Patent granted

1. Ana Mladenovič, Primož Oprčkal, Radmila Milačič, Janez Ščančar, Janja Vidmar, Andrijana Sever Škapin, Peter Nadrah, Alenka Mauko Pranjić, Mirko Šprinzer, Method and system for the potabilization of effluents from biological WWTPS, EP3562788 (B1), European Patent Office, 16. 09. 2020.

INTERNATIONAL PROJECTS

1. CROSSING - Crossing Borders and Scales - An Interdisciplinary Approach
Asst. Prof. Aleš Lapanje
Helmholtz-zentrum Dresden-rossendorf E.v.
2. EMPIR; SIRS - Metrology for Stable Isotope Reference Standards
Prof. Nives Ogrinc
Euramet E.v.
3. ERDF - UIA; APPLAUSE - Alien Plant Species - From Harmful to Useful with Citizens Let Activities
Asst. Prof. Aleš Lapanje
European Regional Development Fund (erdf)
4. EMPIR - EDC-WFD; Metrology for Monitoring Endocrine Disrupting Compounds Under the Water Framework Directive
Prof. Ester Heath
Euramet E.v.
5. LIFE18 ENV/SI; LIFE HIDAQUA
Prof. Radmila Milačič
European Commission
6. EMPIR; STELLAR; Stable Isotope Metrology to enable Climate Action and Regulation
Prof. Nives Ogrinc
Euramet E.v.
7. EMPIR; Si-Hg; Metrology for Traceable Protocols for Elemental and Oxidised Mercury Concentrations
Prof. Milena Horvat
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. COST CA 15202; Self-healing As preventive Repair of COncrete Structures
Asst. Prof. Aleš Lapanje
Cost Association Aisbl
11. 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
12. 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
13. Stability Study of Br in ERM-EC590 and ERM-EC591
Prof. Radojko Jaćimović
European Commission
14. 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
15. Characterization Study of ERM-CZ110
Prof. Radojko Jaćimović
European Commission
16. Training Fees for IAEA"s Fellow Mr Ibrahim Kwame Kwarteng, (GHA0018), 04.11.2019-30.04.2020
Asst. Prof. Branko Kontić
IAEA - International Atomic Energy Agency
17. 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
18. Measurements and Reporting of CRM ERM-CE101 (Ref.: JRC/GEE/2019/VLVP/0056)
Asst. Prof. Tea Zuliani
European Commission
19. Measurements and Reporting of CRMs ERM-CZ120 and BCR-596 (Ref.: JRC/GEE/2020/VLVP/0163)
Asst. Prof. Tea Zuliani
European Commission
20. Training Fees for Hosting Ms. Kasiet Salymbekova, 02.03.2020 - 31.12.2020, ICTP/IAEA STEP Programme
Prof. Milena Horvat
Ictp - Centro Internazionale Di Fisica Teorica
21. COST CA19120 - WATSON; WATer isotopeS in the critical zONe: from groundwater recharge to plant transpiration
Dr. Polona Vreča
Cost Association Aisbl
22. COST CA19145 - SensorFINT; European Network for Assuring Food Integrity Using Non-Destructive Spectral Sensors
Prof. Nives Ogrinc
Cost Association Aisbl
23. COST CA19123 - PHOENIX; Protection, Resilience, Rehabilitation of Damaged Environment
Asst. Prof. Aleš Lapanje
Cost Association Aisbl
24. H2020 -IGOSP; Integrated Global Observing Systems for Persistent Pollutants
Prof. Milena Horvat
European Commission
25. H2020 - ICARUS; Integrated Climate Forcing and Air Pollution Reduction in Urban Systems
Prof. Milena Horvat
European Commission
26. H2020 - HBM4EU; European Human Biomonitoring Initiative
Prof. Milena Horvat
European Commission
27. H2020 - SciShops.eu; Enhancing Responsible and Sustainable Expansion of the Science Shops Ecosystem in Europe
Prof. Milena Horvat
European Commission
28. H2020 - MEET-CINCH; A Modular European Education and Training Concept in Nuclear and RadioChemistry
Asst. Prof. Marko Štrok
European Commission
29. H2020 - NEUROSOME; Exploring the Neurological Exposome
Prof. Milena Horvat
European Commission
30. H2020 - CitieS-Health; Citizen Science for Urban Environment and Health
Dr. David Kocman
European Commission
31. H2020 - HERA; Integrating Environment and Health Research: A Vision for the EU
Prof. Milena Horvat
European Commission
32. H2020 - GREENER; InteGRated systems for Effective ENvironmEntal Remediation
Asst. Prof. Aleš Lapanje
European Commission
33. H2020 - EURAD; European Joint Programme on Radioactive Waste Management
Prof. Milena Horvat
European Commission
34. H2020 - FNS-Cloud; Food Nutrition Security Cloud
Prof. Nives Ogrinc
European Commission
35. H2020 - METROFOOD-PP; METROFOOD-RI Preparatory Phase Project
Prof. Nives Ogrinc
European Commission
36. H2020 - A-CINCH; Augmented Cooperation in Education and Training in Nuclear and Radiochemistry
Asst. Prof. Marko Štrok
European Commission
37. H2020 - GMOS-Train; Global Mercury Observation and Training Network in Support to the Minamata Convention
Prof. Milena Horvat
European Commission
38. H2020 - SurfBio; Innovation Hub for Surface and Colloid Biology Research
Asst. Prof. Aleš Lapanje
European Commission
39. Determination of Geographical Origin of Honey by Using Multi-Element and Isotopic Analysis of Soil, Plants and Honey
Asst. Prof. Tea Zuliani
Slovenian Research Agency
40. Photochemical Fate and Treatment of Pharmaceutical Contaminants in Drinking Water

Asst. Prof. Tina Kosjek
Slovenian Research Agency
41. Mass Balance of Mercury in the Mediterranean Sea
Prof. Milena Horvat
Slovenian Research Agency
42. New Analytical Reference Materials and Techniques for Stable Isotope-Ratio Measurements
Prof. Nives Ogrinc
Slovenian Research Agency
43. Spatial Distribution of d2H, d18O and 87Sr/86Sr in Tap Water and Groundwater from Slovenia
Asst. Prof. Tea Zuliani
Slovenian Research Agency
44. Non-Traditional Isotopes as Novel Tools for Elucidation of Terrestrial Sinks of CO2
Prof. Sonja Lojen
Slovenian Research Agency
45. OrgPlant - Authentication of Organically Grown Plant Products by Novel Stable Isotope Approaches
Prof. Nives Ogrinc
Slovenian Research Agency
46. Radon Mapping and Radon Risk Assessment in Georgia)
Prof. Janja Vaupotič

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. Ligands bearing tzNHCs in Organometallic Chemistry and Homoheneous Catalysis: c-C and C-N Bond Formation in Water
Prof. Ester Heath
2. Closing material flows by wastewater treatment with green technologies
Prof. Ester Heath
3. Mortality of lowland oak forests - consequence of lowering underground water or climate change?
Dr. Polona Vreča
4. Redefinition and revival of copper-free Sonogashira cross-coupling reaction
Prof. Ester Heath
5. Non-traditional isotopes as identifiers of authigenic carbonates
Prof. Sonja Lojen
6. Nanomedicines with antibiotics and probiotics for local treatment of periodontal disease
Asst. Prof. Aleš Lapanje
7. Clinico-pharmacological approach to optimize the therapeutic bleomycin concentration in patients undergoing electrochemotherapy
Asst. Prof. Tina Kosjek
8. Ionom of crop plants for safe and quality food production
Prof. Nives Ogrinc
9. Record of environmental change and human impact in Holocene sediments, Gulf in Trieste
Prof. Sonja Lojen
10. Novel innovative solutions for diaper rash treatment using diapers with probiotic bacteria
Asst. Prof. Aleš Lapanje
11. Methodology approaches in genome-based deversity and ecological plasticity study of truffles from their natural distribution
Prof. Nives Ogrinc
12. Lactic acid fermentation for enrichment of microalgae biomass with new nutrients
Prof. Nives Ogrinc
13. 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
14. 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
15. Indentifying the genetic determinants of chemical toxicity in the green alga Chlamydomonas reinhardtii
Prof. Milena Horvat
16. Bisphenol A alternatives: transfer from food contact material, fate and human exposure
Prof. Ester Heath
17. Stable isotopes in the study of the impact of increasing CO2 levels on C and Hg cycling in coastal waters
Prof. Nives Ogrinc
18. Neuropsychological dysfunctions caused by low level exposure to selected environmental pollutants in susceptible population – NEURODYS
Prof. Milena Horvat
19. BE MERMAiD - Bioavailable mercury methylation in the Adriatic sea
Prof. Milena Horvat
20. STRAP - Sources, TRansport and fate of persistent Air Pollutants in the environment of Slovenia
Prof. Nives Ogrinc
21. Novel approaches for the estimation of the use of psychoactive pharmaceuticals and illicit drugs by wastewater analysis
Prof. Ester Heath
22. Novel proxies of the Holocene climate variability in stalagmites in Slovenia
Prof. Sonja Lojen
23. Cost-efficient separation of tritium from water with bio-based systems – BIOTRISEP
Asst. Prof. Marko Štrok
24. Influence of geotechnical fills from recycled materials on groundwater
Prof. Radmila Milačič
25. EcoFAR: Food security and climate change mitigation by means of ecological farming development - conservation tillage, bioeffectors and sustainable weed management
Prof. Nives Ogrinc
26. Photocatalytic water treatment - development of immobilized catalysts and compact reactor systems
Prof. Ester Heath
27. Illict drugs, alcohol and tobacco: wastewater based epidemiology, treatment efficiency and vulnerability assessment of water catchments
Asst. Prof. Tina Kosjek
28. Identification of Pb sources in the upper Mežiška valley based on Pb isotope composition
Asst. Prof. Tea Zuliani
29. Food for future - F4F
Prof. Nives Ogrinc
Ministry of Education, Science and Sport
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. Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF)
Prof. Nives Ogrinc
Ministry of Economic Development and Technology
35. Pursuing authenticity and valorization of Mediterranean traditional products
Prof. Nives Ogrinc
Ministry of Education, Science and Sport
36. Molybdenum geobiochemical Cycle in modern environments
Prof. Sonja Lojen
Slovenian Research Agency
37. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
Prof. Milena Horvat
Slovenian Research Agency
38. Implementation of the Human Biomonitoring program 2018-2022
Prof. Milena Horvat
Ministry of Health
39. Implementation of official sample analyses activities for 2020
Prof. Nives Ogrinc
Ministry of Agriculture, Forestry and Food
40. Identification of Pb sources in the upper Mežiška valley based on Pb isotope composition
Asst. Prof. Tea Zuliani
Slovenian Research Agency
41. Identification of Pb sources in the upper Mežiška valley based on Pb isotope composition
Asst. Prof. Tea Zuliani
Ministry of Health
42. Services; Determination of the Isotopic Composition of Carbon in Sugar Samples
Prof. Nives Ogrinc
43. Different Analyses
Prof. Sonja Lojen

44. Small Services
Dr. Tjaša Kanduč
45. Small Services in the Year 2021
Prof. Milena Horvat
46. Analyses of Metals, TBT and DBT in Sediments, Mussels and Fish
Prof. Janez Ščančar
47. HGKYR - Measurements of Elements in Environmental and Biological Samples from Kyrgyzstan
Prof. Milena Horvat
Médecins Sans Frontieres, Representation Of
48. 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, Center For
49. 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 of
50. Dual (Oxygen and Strontioum) Stable Isotope-Based Wood Provenancing
Asst. Prof. Tea Zuliani
Stefan Cel Mare University of Suceava

NEW CONTRACTS

1. Measurements of gaseous effluents, specific analysis of H-3 and C-14 in year 2020
Asst. Prof. Marko Štrok
Nuklearna Elektrarna Krško d. o. o.
2. National monitoring of radioactivity in the environment in the Republic of Slovenia for 2020
Asst. Prof. Marko Štrok
Ministry of the Environment and Spatial Planning
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. Marko Štrok
Nuklearna Elektrarna Krško d. o. o.
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. Marko Štrok
Nuklearna Elektrarna Krško d. o. o.
5. Analyses of tributyl and dibutyltin compounds in water and biota in 2020
Asst. Prof. Tea Zuliani
Ministry of the Environment and Spatial Planning
6. Monitoring of radioactivity in drinking water for years 2020 and 2021 (lot 2)
Asst. Prof. Marko Štrok
Ministry of Health
7. Qualitative and quantitative monitoring of groundwater in the impact area of the dam for HPP Mokrice
Dr. Tjaša Kanduč
Irgo Consulting d. o. o.
8. Measurements of mercury in air and precipitation for 2021 and 2022
Prof. Milena Horvat
Ministry of the Environment and Spatial Planning

VISITORS FROM ABROAD

1. Ivna Vrana Špoljarić, Ruđer Bošković Institute, Zagreb, Croatia, 15 September 2019 to 15 September 2020
2. Neri Bonciani, Universita degli studi di Firenze, Firenze, Italy, 1 November 2019 to 20 August 2020
3. Ibrahim Kwame Kwarteng, Ghana Atomic Energy Commision, Accra, Ghana, 4 November 2019 to 9 August 2020
4. Bright Birikorang, School of Nuclear and Allied Sciences, Accra, Ghana, 27 January to 31 December 2020
5. Maaire Gyengne Francis, Lawra Methodist Junior High School, Accra, Ghana, 27 January to 31 December 2020
6. dr. Alexander Rudloff, International Union of Geodesy and Geophysics (IUGG), Potsdam, Germany, 29–30 January 2020
7. dr. Alexandre Soares Leal, Centre for Development of Nuclear Technology, Belo Horizonte, Brazil, 1 February to 11 March 2020
8. prof. dr. Gleb Sukhorukov, School of Engineering and Materials Science, Queen Mary, University of London, London, United Kingdom, 14–15 February 2020
9. dr. Dominika Saniewska, Institute of Oceanography, University of Gdańsk, Gdańsk, Poland, 1–20 March 2020
10. Kasiet Salymbekova, Ministry of Health of the Kyrgyz Republic, Bishkek, Kyrgyzstan, 2 March to 10 August 2020
11. dr. Hanns Moshammer, Medical University of Vienna, Austria, 30 June 2020
12. Miroslav Vanek, Technical University in Zvolen, Zvolen, Slovakia, 30 August to 5 September 2020

STAFF

Researchers
1. Prof. Ljudmila Benedik
2. Asst. Prof. Ingrid Falnoga
3. Dr. David John Heath
4. Prof. Ester Heath
5. **Prof. Milena Horvat, Head**
6. Prof. Radojko Jaćimović
7. Dr. Tjaša Kanduč
8. Dr. David Kocman
9. *Asst. Prof. Branko Kontić, retired 01.09.20*
10. Asst. Prof. Tina Kosjek
11. Asst. Prof. Jože Kotnik
12. Asst. Prof. Aleš Lapanje
13. Prof. Sonja Lojen
14. Dr. Darja Mazej
15. Prof. Radmila Milačič
16. Prof. Nives Ogrinc
17. Asst. Prof. Tomaž Rijavec
18. Prof. Borut Smodiš
19. Prof. Janez Ščančar
20. Asst. Prof. Zdenka Šlejkovec
21. Asst. Prof. Marko Štrok
22. Prof. Janja Vaupotič
23. Dr. Janja Vidmar
24. Dr. Polona Vreča
25. Asst. Prof. Tea Zuliani
26. Dr. Dušan Žigon

Postdoctoral associates
27. Ermira Begu, B. Sc.
28. Raghuraj Singh Chouhan, B. Sc.
29. Dr. Marta Jagodic Hudobivnik
30. Asst. Prof. Davor Kontić
31. Dr. Bor Krajnc
32. Dr. Doris Potočnik
33. Janja Snoj Tratnik, B. Sc.
34. Dr. Anja Stajnko
35. *Dr. Ajda Trdin, left 16.11.20*
36. Dr. Igor Živković

Postgraduates
37. Teodor-Daniel Andron, B. Sc.
38. Tine Bizjak, B. Sc.
39. Dominik Božič, B. Sc.
40. *Jutra Černilogar Mrzelj, B. Sc., left 07.03.20*
41. Jan Gačnik, B. Sc.
42. Tjaša Goltnik, B. Sc.
43. *Tjaša Gornik, B. Sc., left 01.09.20*
44. Ana Kovačič, B. Sc.
45. Katarina Marković, B. Sc.
46. Jasmina Masten Rutar, B. Sc.
47. Klara Nagode, B. Sc.
48. Rok Novak, B. Sc.
49. Johanna Amalia Robinson, B. Sc.
50. Leja Rovan, B. Sc.
51. Agneta Annika Runkel, B. Sc.
52. Lidija Strojnik, B. Sc.
53. Žiga Tkalec, B. Sc.
54. Maja Zugan, B. Sc.

Technical and administrative staff
55. Barbara Svetek, B. Sc.
56. Karolina Trentelj, B. Sc.
57. Zdenka Trkov, B. Sc.
58. Vanja Usenik, B. Sc.
59. Tina Vrabec, B. Sc.
60. Stojan Žigon

BIBLIOGRAPHY

Original Article

1. Sabina Berisha, Igor Živković, Jože Kotnik, Tanja Ljubič-Mlakar, Milena Horvat, "Quantification of total mercury in samples from cement production processing with thermal decomposition coupled with AAS", *Accreditation and quality assurance*, 2020, **25**, 3, 233–242.
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5. Ajda Trdin, *Mercury speciation in prenatal exposure:* doctoral dissertation, Ljubljana, 2020 (mentor Milena Horvat; co-mentor Ingrid Falnoga).

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 intelligent control, humanoids, cognitive robotics, robot learning 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 optimising "the behaviour of man and machine", accounting for interactions with the environment. By combining engineering and life sciences, we have been able to make breakthrough contributions in the area 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.

Head:
Prof. Aleš Ude

The department maintains the programme group "Automation, robotics and biocybernetics" in the field of Production Technologies (leader prof. dr. Igor B. Mekjavic). Members of the department participate in numerous EU projects in the area of robotics and artificial intelligence, factories of the future, health, and space technologies. In 2020 we coordinated one Horizon 2020 project, ReconCycle. We are also active in transferring our research results to various applications through direct collaboration with industry.

Research in the area of humanoid robotics and robot learning is primarily conducted within the Humanoid and Cognitive Robotics Lab (leader dr. Bojan Nemec), which operates within the department. The aim of this laboratory is to create robots that are capable of acquiring new knowledge through learning and to collaborate with people in their natural environments. Another laboratory that operates within the department is Laboratory for Neuromechanics and Biorobotics, which is led by prof. dr. Jan Babič. The main focus of this lab is to integrate the results of biomechaniscs, neurophysiology and robotics to study human motor control and develop new robot systems that can effectively assist people in their daily activities.

By maintaining a critical mass of researchers in the area of robotics, automation and life sciences within one department, we have managed to foster exciting multidisciplinary projects.

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.

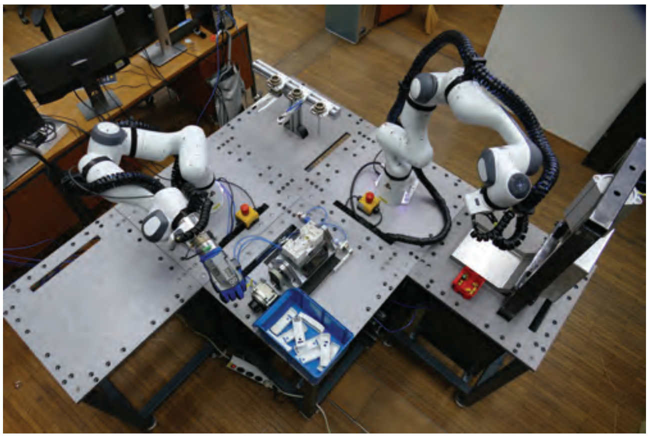

Figure 1: Reconfigurable cell for the recycling of electronic devices

Robotics

In 2020 we launched a new Horizon 2020 project **ReconCycle** (Self-reconfiguration of a robotic workcell for the recycling of electronic waste, http://www.reconcycle.eu/), which we also coordinate. 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 in the ReconCell project, http://www.reconcell.eu/. The challenge is to provide methodologies for the re-design of the recycling cell,

In the H2020 project ReconCycle we aim to substantially reduce human effort and increase the accuracy and efficiency of recycling.

Figure 2: Basic module for the construction of reconfigurable robotics cells

including the location of robots and other elements in the workcell and the choice of grippers and sensing systems. On the software side, approaches for 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 in 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 desired task.

We continued working 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 2020 we developed an approach for the efficient incremental learning from demonstration, aiming to directly modify the robot motion parameters by human instruction. We have proven its learning stability and evaluated the proposed framework with a comprehensive user study. Another important result was a proposal for the automated optimization of collaborative workspaces with respect to the capabilities of robots and human workers.

To decisively improve the process of skill learning needed to realize advanced production tasks in ReconCycle and CoLLaboratE, we developed a new approach for learning sensorimotor skills represented by **dynamic movement primitives** using **deep neural networks**. The distinguishing property of our approach is that it can utilize loss functions that measure the physical distance between robotic operations and thus improves the quality of the learnt skills. While the developed approach is applicable to any neural network's architecture, it was first evaluated on two different architectures based on encoder–decoder networks and convolutional neural networks. In the follow-up research we have shown that the proposed approach can also improve the training of deep recurrent neural networks, which is important when processing time-variant sensory data.

In the H2020 project AnDy we work on endowing robots with the ability to control physical collaboration through intentional interaction.

In the scope of the Horizon 2020 project **AnDy** (https://andy-project.eu) we continued our work to implement and evaluate different exoskeleton solutions in industrial settings. After **successful experimentation of the passive shoulder exoskeleton in the car production** company Revoz, we moved on to the implementation of the active shoulder exoskeleton that will further expand the range of use of such devices in the real-world industrial applications. We assembled an experimental lab setup to test the feasibility of different robotic controllers that can be utilized in the active exoskeletons and prepared a quantifiable set of matrices that we will use for its evaluation. In parallel with the exoskeleton implementation and evaluation, we continued our work in the domain of human–human collaboration with the aim to unravel the information flow between a group of human subjects during collaborative motor task execution. The results will be formalized and modelled with the aim to implement them in future exoskeleton controllers and collaborative robots.

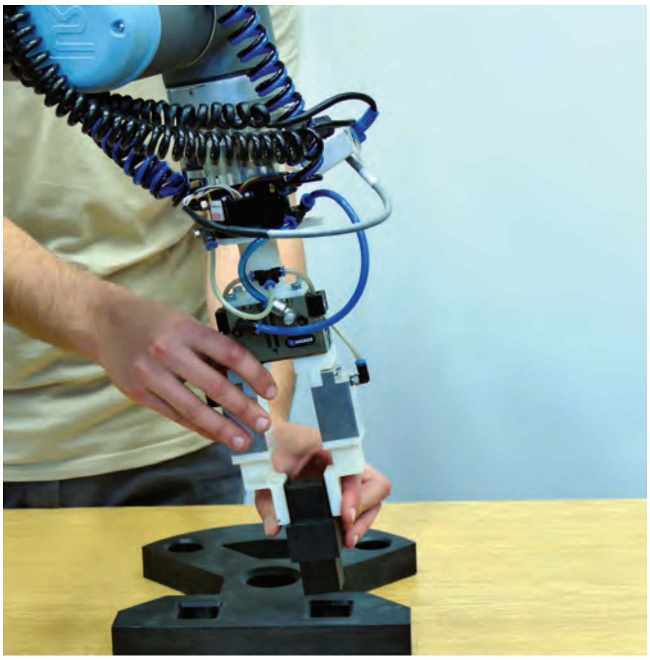

Figure 3: Incremental teaching of robot operations

In the scope of **EXOSAFE**, which was carried out as part of the Horizon 2020 COVR project, we designed, developed and built a bionic human leg that will be used in the benchmarking of lower-leg exoskeletons. The bionic leg is in the process of being patented.

Under the Director's Fund project **Cobotat** (Laboratory for Advancing Collaborative Robot Behaviors in Physical Human-Robot Interaction Scenarios, http://cobotat.ijs.si/) we continued to work on the construction of new laboratory facilities. The main work focused on the integration of motion capture, force plates and electromyographic sensors. Linked to the developments in the CoBoTaT lab, we continued to work on two projects funded by Slovenian Research Agency: **PhRoCiety** (Collaborative Capabilities in Physical Human-Robot Interaction Scenarios, http://cobotat.ijs.si/projects/phrociety-2/) and **SWITCH** (Learning by Switching Roles in Physical Human-Robot Collaboration, https://switch-project.github.io/), which is co-funded by SNFS. The goal of the PhRoCiety project is to advance the cognitive understanding and current control of cooperative and robust physical multi-contact interaction between multiple agents, where the agents are humans or robots. To this end, we have conducted several laboratory studies, **investigating physical human-human interaction**. The main goal of SWITCH is to improve physical human-robot collaboration by developing methods that can efficiently observe human dynamics in real time and learn anticipatory models from a demonstration. Here, we aim to collect multiple datasets of force and motion capture data for a human-human stand-up task. We will then develop models that can learn the behaviour of the two agents (assistant and assisted) in a probabilistic manner. These models will be used for the **online control of robots with reactive and anticipatory capabilities**.

Work is under way to establish a new experimental lab Cobotat – Laboratory for Advancing Collaborative Robot Behaviors in Physical Human-Robot Interaction Scenarios.

The main objective of the **TRINITY** project (https://trinityrobotics.eu/), another Horizon 2020 project in our department, is to create a network of multidisciplinary and synergistic local digital innovation hubs (DIHs) composed of research centres, companies, and university groups that cover 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 to support the introduction of advanced robotic systems in the production processes. In 2020 we have newly implemented demonstrators that show **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. We expect that the modules from our demonstrators will be offered to the manufacturing SMEs within a TRINITY open call.

In **QU4LITY** (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. In 2020 we collaborated with the Slovenian company Kolektor and developed a cell at the end of the moulding line for visual quality inspection. The cell will enable new robot-supported approaches to visual quality inspection based on deep learning and automated workcell reconfiguration technologies.

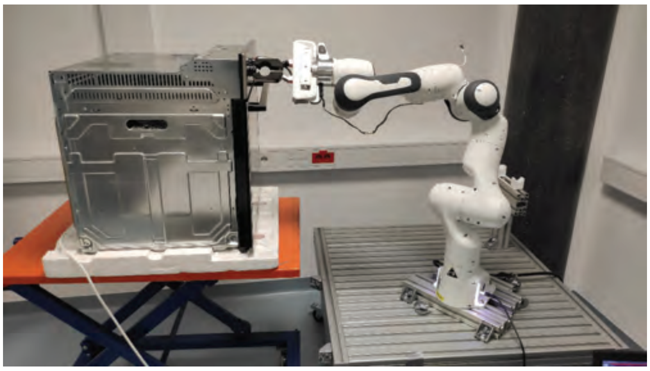

Figure 4: Testing of ovens for quality control

Automation and robotics in industrial production processes

An important part of this work was the implementation of the GOSTOP Program (Buildings, Tools and Systems for the Factories of the Future), which was **coordinated** by our department (dr. Igor Kovač) and successfully completed in 2020. The Program GOSTOP was the biggest research/development programme in Slovenia in the field of Factories of the Future. Its aim was to accelerate the design and development of the factories-of-the-future concept in Slovenia and to provide solutions for the current needs of Slovenian industry, where some companies have already started to introduce this concept into their production facilities. We identified four areas in which decisive breakthroughs can be achieved in Slovenia in the near future: control technologies, tooling, robotics, and photonics. In the area of robotics, we collaborated with companies such as Kolektor, Domel, Yaskawa, and Podkrižnik.

The three-and-a-half-year program GOSTOP involved 19 partners from 13 Slovenian companies and 6 research organizations and resulted in 17 patents and 40 innovations.

In GOSTOP our group successfully addressed the following topics: 1. **intelligent sensors and actuators**, 2. **adaptive robotic workcell for visual quality control**, and 3. **platform of the virtual factory**. Research in the area of intelligent sensors and actuators resulted in an intelligent drive assembly that provides accurate positioning and allows monitoring of drive parameters and their evaluation to predict maintenance. In the second research theme, i.e., adaptive robotic workcell, we contributed to the development of an adaptive robotic cell for applications in visual quality control. The main goal of the development of a virtual factory platform was to design and produce an intelligent, competitive and sustainable information system in a smart factory that includes the elements of robotics.

A vital mission of our department is the transfer of our research results to industrial applications. In past 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 Slovenian industry. The key achievements of SRIP FoF in 2020 were the preparation of a new program to foster the cooperation of manufacturing companies with the research departments at the universities and institutes and transfer our latest research results into industrial practice.

Also in the scope of the Slovenian Smart Specialization Strategy, we have joined the **ROBKONCEL** project, whose main goal is to develop a

Figure 5: Cobotat laboratory with mobile robots

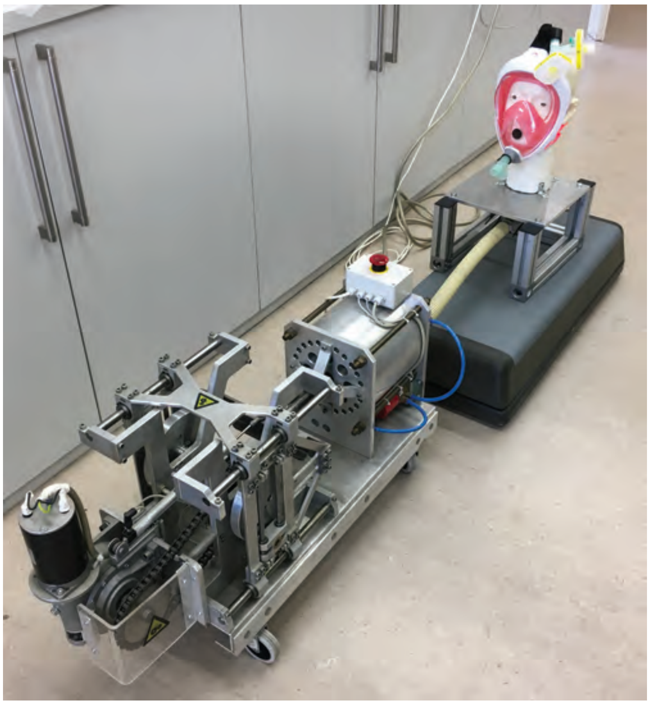

Figure 6: Evaluation of masks using the head manikin and breathing simulator

comprehensive system for quality control in the production processes and inspection of finished products. In 2020 **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 Franka Emika Panda, whereas Universal robots UR10 robots were used to implement the forging control cell for Unior. We have developed an appropriate software environment for the programming of collaborative robots, which supports modern concepts of robot learning techniques. We have also proposed new approaches that improve the flexibility and adaptability to product changes and inspection procedures. One of the goals of demonstration cells is to allow the evaluation of the functionality that the final cell must provide. An important aspect is also an indicative cost estimate of individual functionalities in the final stage.

In collaboration with a Slovenian company Podkrižnik, we carried out **S-Gearbox Ultra** project. The aim of the project was to upgrade the S-Gearbox product with the ability to measure torque. Such gearboxes are rapidly being introduced in robotics and related applications. **Transmissions with integrated torque sensors** are essential to perform collaborative tasks in which a robot must accurately adapt to a human and its environment. In the course of the project, we performed a detailed analysis that served as a basis to design and build several different prototypes of the torque-sensor system. We performed numerous tests to select the most suitable design.

Environmental physiology and ergonomics

The unfortunate occurrence and global spread of the severe acute respiratory syndrome corona virus 2 (SARS-CoV-2) resulted in the Covid-19 pandemic in 2020. As a consequence, an added focus of our work was to provide assistance to our clinical and industrial partners in developing and evaluating personal protective equipment.

Infrared thermography to screen for Covid-19 and other infections: Around the planet, in many different scenarios, skin temperature is being used as a surrogate measure of deep body (core) temperature in the assessment of whether an individual is infected with the SARS-CoV-2, which causes Covid-19, as indicated by the presence of fever. The key question is whether or not this is a valid methodology? If it is not, we run the risk of falsely excluding individuals from places they may want, or need, to go. We also run the risk of falsely allowing people into places where they can spread the undetected infection they have. We initiated a programme of research to **evaluate the method of predicting deep body (core) temperature** using infrared thermography from measurements of the forehead's skin temperature.

Personal protective clothing: Building on the knowledge and experience of previous collaborative projects with the industrial partner Kimberly-Clark (USA) evaluating disposable personal protective garments used in the manufacturing industry, we continued this collaboration by establishing a standardised test protocol to evaluate the work of breathing imposed on the wearer by face masks. Together with colleagues from the Department of Condensed Matter Physics (F5), we established a test utilising a head manikin to evaluate the particle removal efficiency of masks, where the size of the particles was in the same range as the size of the coronavirus. Over 100 masks were tested for industrial partners in this manner. Due to the urgent need for face masks by healthcare workers, several strategies for disinfecting and reactivating used masks have been evaluated in collaboration with the Reactor Physics Department (F8).

A system for testing protective masks using a head manikin and breathing simulator has been developed.

Cooling vests: The 21st century has posed challenges to the survival of the human race, such as global warming. As a consequence of global warming, summer heat waves have increased in frequency, duration and intensity. In the H2020 project **Heat-Shield**, one of our tasks is the evaluation and development of strategies to mitigate occupational heat strain during such heat waves in key European industries. We developed a test using a sweating thermal manikin to evaluate the efficacy of cooling vests. With this experimental method, we evaluated cooling vests with different cooling concepts, including active air- or water-cooling vests, evaporative vests, vests using phase-change material inserts (PCM) and hybrid vests. The key finding of the study was that under the given ambient conditions (Ta = 35 °C, RH = 35 %) cooling capacities differed significantly among different vests and cooling concepts. Our report provides managers in industry with guidelines for how to choose appropriate vests for their workers.

Heat-wave simulation: Despite the significant impact of summer heat waves on the health and well-being of workers, there has been no controlled laboratory study to date that would provide data regarding the effect of a prolonged exposure to simulated heat-wave conditions on labour productivity. Previously, we reported that productivity in a manufacturing company can decline for a short period (i.e., 3 days) even after the cessation of a heat wave. We reasoned that this could be due to a cumulative effect of heat waves, indicating that the recovery from a heat wave required some time. During periods of heat waves, workers can be exposed to heat also during their time at home, meaning they may not be able to recover properly. We established a **simulation of a 3-day heat wave** in the Olympic Sport Centre Planica, where we run the PlanHab facility. Participants were exposed to a 3-day period of a normal temperature environment, proceeded by a 3-day heat wave, and ending with a 3-day normal temperature environment. During each day, participants conducted a simulated 8-hour work-shift incorporating two 40-minute moderate-intensity sessions, followed by a 1-hour light-intensity assembly-line task. The simulated heat wave increased the number of mistakes made, time spent on unplanned breaks, and the physiological strain experienced by the participants. Overall, the simulated heat wave caused a significant reduction in labour productivity and increase in physiological strain.

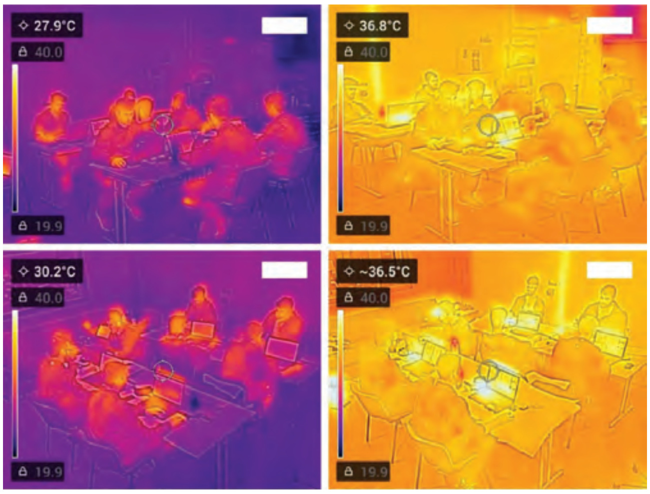

Figure 7: Ambient conditions during the day prior to the heat wave (left) and the first day of the heat wave (right)

Space-flight associated neuro-ocular syndrome: Two, as yet unresolved, issues have jeopardised future deep-space exploration missions by humans. One is the effect of radiation to which humans are exposed in space and our current inability to provide adequate protection of astronauts from the detrimental effects of this radiation. The other issue is the unexplained ophthalmic changes observed in astronauts during long (several month) missions on the International Space Station (ISS). These ophthalmic changes have been termed the **Space-flight Associated Neuro-ocular Syndrome** (SANS). We have initiated a programme of research to identify the factors that might contribute to SANS. Our results demonstrate that the current approach of conducting eye examinations in the supine horizontal or head down tilt position is not appropriate, as it does not initiate the changes in intraocular pressure observed in space. Our continued goal is to evaluate the effects of age, gender, exercise, hypoxia and hypercapnia on intraocular, and possibly intracranial pressures.

Our group has been given an opportunity by ESA to install a short-arm human centrifuge.

Short-arm human centrifuge: ESA has embarked on a new research programme, which will investigate the utility of implementing artificial gravity during future deep-space missions. For this purpose, it has developed short-arm human centrifuges, which will be used in three research centres in Europe to test the efficiency of artificial gravity in mitigating the microgravity-induced changes, particularly in the musculoskeletal and cardiovascular systems. The programme will also investigate the inclusion of exercise during the daily centrifugation. We have been selected **by ESA to operate one of the short-arm human centrifuges** in the PlanHab facility in Planica. This will provide us with an opportunity to initiate a programme of research into the benefits of resistance vibration exercise combined with artificial gravity in mitigating the known adaptations to microgravity An additional aim is to assess whether hypoxia modifies the mitigation of microgravity-induced alterations in the adaptive processes.

Some outstanding publications in the past year

1. T. Gašpar, M. Deniša, P. Radanovič, B. Ridge, T. R. Savarimuthu, A. Kramberger, M. Priggemeyer, J. Roßmann, F. Wörgötter, T. Ivanovska, S. Parizi, Ž. Gosar, I. Kovač, and A. Ude (2020) Smart hardware integration with advanced robot programming technologies for efficient reconfiguration of robot workcells, Robotics and Computer-Integrated Manufacturing, vol. 66, art. 101979, pp. 1-17.
2. M. Jamšek, T. Petrič, and J. Babič (2020) Gaussian mixture models for control of quasi-passive spinal exoskeletons, Sensors, vol. 20, art. 2705, pp. 1-13.
3. U. Ciuha, S. N. Kounalakis, A. McDonnell, and I. B. Mekjavić (2020) Seasonal variation of temperature regulation: do thermoregulatory responses “spring” forward and “fall” back?, International Journal of Biometeorology, vol. 64, pp. 1221-1231.
4. R. Pahič, B. Ridge, A. Gams, J. Morimoto, and A. Ude (2020) Training of deep neural networks for the generation of dynamic movement primitives, Neural Networks, vol. 127, pp. 121-131.
5. T. Petrič (2020) Phase-synchronized learning of periodic compliant movement primitives (P-CMPs), Frontiers in Neurorobotics, vol. 14, art. 599889, pp. 1-12.
6. A. Sotiridis, U. Ciuha, T. Debevec, and I. B. Mekjavić (2020) Heat acclimation does not modify autonomic responses to core cooling and the skin thermal comfort zone, Journal of Thermal Biology, vol. 91, art. 102602, pp. 1-8.

Awards and Appointments

1. Tim Podlogar: Gatorade Sports Science Institute Award, Köln, Germany, 25. ECSS Congress European College of Sport Science (virtual), Effectiveness of combined galactose-glucose ingestion as compared to galactose or glucose only on post-exercise muscle glycogen repletion

Organization of conferences, congresses and meetings

1. Kickoff meeting of ReconCycle project, Jožef Stefan Institute, Ljubljana, 13. - 14. 2. 2020.
2. Final review meeting of H2020 Spexor project, 23.-24.3.2020 (virtual)
3. Workshop "Human Movement Understanding for Intelligent Robots and Systems", https://iros2020hmu.wixsite.com/website, IROS 2020, Las Vegas, USA, 25. 10. 2020 (held via videoconference because of Covid-19).
4. General meeting of H2020 ReconCycle project, 27.11.2020 (virtual)

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. Palmer Study
   Prof. Igor Mekjavić
   W. L. Gore & Associates Gmbh
3. Tests of Rt and Re of 5 Insole-Shoe Combinations
   Prof. Igor Mekjavić
   Geox S.p.a.
4. COST CA16116 - 20786; Wearable Robots for Augmentation, Assistance or Substitution of Human Motor Functions
   Prof. Jan Babič
   Cost Office
5. ESA - Individual Variation in Human Response to prolonged Bed Rest in Slovenia Bed Rest Programme
   Prof. Igor Mekjavić
   Esa/estec.
6. COST CA16116 - 20786; Review Panel Meetings
   Prof. Jan Babič
   Cost Association Aisbl
7. COST CA16116 - 20786; Review Panel Meetings
   Prof. Jan Babič
   Cost Association Aisbl
8. 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
9. H2020 - An.Dy; Advancing Anticipatory Behaviors in Dyadic Human-Robot Collaboration
   Prof. Jan Babič
   European Commission
10. H2020 - CoLLaboratE: Co-production CeLL performing Human-RobotCollaborative AssEmbly
    Prof. Bojan Nemec
    European Commission
11. H2020 - TRINITY; Digital Technologies, Advanced Robotics and increased Cyber-Security for Agile Production in Future European Manufacturing
    Prof. Aleš Ude
    European Commission
12. H2020 - QU4LITY; Digital Reality in Zero Defect Manufacturing
    Prof. Aleš Ude
    European Commission
13. H2020 - COVR: EXOSAFE; A Mechatronic Leg Replica to Benchmark Human-Exoskeleton Interaction
    Prof. Jan Babič
    European Commission
14. H2020 - ReconCycle; Self-reconfiguration of a Robotic Workcell for the Recycling of Electronic Waste
    Prof. Aleš Ude
    European Commission
15. Learning Cross-Task Generalization for Model-Predictive Control: Application to Dynamic Humanoid Behaviors
    Prof. Andrej Gams
    Slovenian Research Agency
16. The Interaction of Regional Thermal and Baroreflex Regulation of the Peripheral Circulation
    Prof. Igor Mekjavić
    Slovenian Research Agency
17. Generation and Learning of Adaptive Cyclic Movements in Assist-As-Needed Applications for Human-Robot Interaction
    Asst. Prof. Tadej Petrič
    Slovenian Research Agency

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. 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
7. Building blocks, tools and systems for the Factories of the Future – GOSTOP
   Asst. Prof. Igor Kovač
   Ministry of Education, Science and Sport
8. Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF)
   Asst. Prof. Igor Kovač
   Ministry of Economic Development and Technology
9. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
   Prof. Aleš Ude
   Slovenian Research Agency
10. Stimulators and Parts
    Prof. Aleš Ude
11. TRUExo - Implementation of an Exoskeleton for the Torso in the Rehabilitation Process of Patients with Multiple Myeloma
    Prof. Jan Babič
    Istituto Nazionale Tumori, Centro Di Riferimento
12. Mitten Testing
    Prof. Igor Mekjavić
    Ministry of Defence
13. ALITO: Testing of Face Masks
    Prof. Igor Mekjavić
    Kimberly-Clark

NEW CONTRACT

1. LAMA: Development of a new machine concept
   Asst. Prof. Igor Kovač
   Lama Avtomatizacija d. o. o.

VISITORS FROM ABROAD

1. Riccardo Persichini, qbrobotics srl, Pisa, Italy, 13.-14.2.2020
2. Minija Tamosiunaite, Göttingen University, Germany, 13.-14.2.2020
3. Florentin Wörgötter, Göttingen University, Germany, 13.-14.2.2020
4. Saeed Abdolshah, Technische Universität München, Germany, 13.-14.2.2020
5. Erfan Shahriari, Technische Universität München, Germany, 13.-14.2.2020
6. Hanes Frolich, ElectroCycling GMbH, Germany, 13.-14.2.2020
7. Giorgio Grioli, Italian Institute of Technology (IIT), Italy, 13.-14.2.2020
8. Vinicio Tincani, Italian Institute of Technology (IIT), Italy, 13.-14.2.2020
9. Manuel Catalano, Italian Institute of Technology (IIT), Italy, 13.-14.2.2020
10. Lydia Tsoutsoubi, University of Thessaloniki, Greece, 11.-21.9.2020
11. Mantzios Konstantinos, University of Thessaloniki, Greece, 11.-21.9.2020
12. Zoe Panagiotaki, University of Thessaloniki, Greece, 11.-21.9.2020
13. Areti Kapnia, University of Thessaloniki, Greece, 11.-21.9.2020

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4. Prof. Polonca Jaki Mekjavić*
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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*
13. **Prof. Aleš Ude, Head**
14. Asst. Prof. Leon Žlajpah

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17. Dr. Urša Ciuha
18. Dr. Jernej Čamernik
19. Dr. Miha Deniša
20. Dr. Miha Dežman
21. Leonidas Ioannou, B. Sc.
22. Dr. Tim Podlogar
23. *Dr. Barry Martin Ridge, left 15.02.20*
24. Desy Salvadego, B. Sc.

Postgraduates
25. Jason Thomas Fisher, B. Sc.
26. Timotej Gašpar, B. Sc.
27. Marko Jamšek, B. Sc.
28. Jaka Jereb, B. Sc.
29. Tjaša Kunavar, B. Sc.
30. Zvezdan Lončarević, B. Sc.
31. Matija Mavsar, B. Sc.
32. Luka Mišković, B. Sc.
33. Tinkara Mlinar, B. Sc.
34. Benjamin Jonathan Narang, B. Sc.
35. Rok Pahič, B. Sc.
36. Joshua Toby Royal, B. Sc.
37. Mihael Simonič, B. Sc.

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38. Tanja Dragojević, B. Sc.
39. Mitja Gliha, B. Sc.
40. *Daša Gorjan, B. Sc., left 01.10.20*
41. *Gregor Klinc, B. Sc., left 01.03.20*
42. Rebeka Kropivšek Leskovar, B. Sc.
43. Matevž Majcen Hrovat, B. Sc.
44. Primož Radanovič, B. Sc.
45. Simon Reberšek, B. Sc.
46. *Manca Stare*, B. Sc., left 01.11.20*
47. Matej Štefanič, B. Sc.
48. Andrej Trošt, B. Sc.
49. *Tamara Valenčič, B. Sc., left 21.09.20*
50. Bogomir Vrhovec, B. Sc.

Technical and administrative staff
51. *Željka Kukec, B. Sc., left 01.04.20*
52. Petra Movh, B. Sc.
53. *Danijela Zeljković Anžiček, B. Sc., left 01.11.20*

Note:

* part-time JSI member

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Independent Component Part or a Chapter in a Monograph

1. Tatsuya Teramae, Koji Ishihara, Jan Babič, Jun Morimoto, Erhan Oztop, "Human-in-the-loop control and task learning for pneumatically actuated muscle based robots", In: *Human-in-the-loop robot control and learning*, (Frontiers research topics), Frontiers Media, 2020, 209-217.

Theses and Mentoring

1. Jernej Čamernik, *Postural control in response to external perturbations: biomechanics of extended support:* doctoral dissertation, Ljubljana, 2020 (mentor Jan Babič).
2. Miha Dežman, *Applications of passive and mechanically variable stiffness elements in wearable robotic mechanisms:* doctoral dissertation, Ljubljana, 2020 (mentor Andrej Gams).
3. Timotej Gašpar, *Technologies for fast reconfiguration of adaptive robotic workcells:* doctoral dissertation, Ljubljana, 2020 (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 to support the design of control systems, the development of specific measurement and control modules, and the development and construction of complete systems for the control and supervision of machines, devices and industrial processes.

Head:

Asst. Prof. Gregor Dolanc

Basic and applied research in 2020 was devoted to three sub-areas: methodologies for analysis and control systems design; tools and building blocks for implementation; and applied research in the priority problem domains.

The first topic addressed the ***modelling and identification of nonlinear and complex dynamical systems***. Research activities were pursued in the direction of hybrid modelling with Gaussian-process models as well as modelling with entirely data-driven methods. The methods were utilised for the modelling of atmospheric humidity, wastewater treatment plants and in medicine. We also participated in the research of automatic equation discovery.

We have continued the research and development of model-predictive-control methods based on fast online optimization. We have implemented the algorithm of the primal-fast-gradient method, used in a challenging multivariable control scheme for the stabilization of the unstable resistive wall modes for the ITER tokamak fusion reactor, with a high-level synthesis approach for FPGA programming using fixed-point arithmetic. The achieved computation time of 0.011 ms is an order of magnitude shorter than the one previously achieved using a standard processor.

In the field of smart factories, we were active in three main areas: (i) product quality management, (ii) development of algorithms for monitoring and evaluation of the operators' actions, and (iii) development of algorithms for event detection from continuous process measurements. Within the first two areas, an approach was developed for SIJ ACRONI, where on the basis of a past operator's corrective actions, conclusions are made on when and how to adjust the recipe to achieve better product quality (Figure 1). Event-detection analyses were performed as a study focused on the development of a system for the non-invasive monitoring and diagnostics of repetitive production processes.

Figure 1: Control room in SIJ Acroni d.o.o. (photo: Arhiv SIJ Acroni)

During the final phase of our bilateral project with CEA, Grenoble, France, in 2020, the two-dimensional (2-D), microstructural SOFC model was validated. The key feature of the model embraces the degradation of the SOFC's voltage due to the nickel (Ni) agglomeration that occurs at high operational temperatures. Based on periodic measurements during the first 1000 hours the model parameters were fitted to calculate the voltage profile over the time of 10,000 hours by using the model (Figure 2). Such an approach is useful to assess the lifetime of SOFC and related cost per kWh of electric energy.

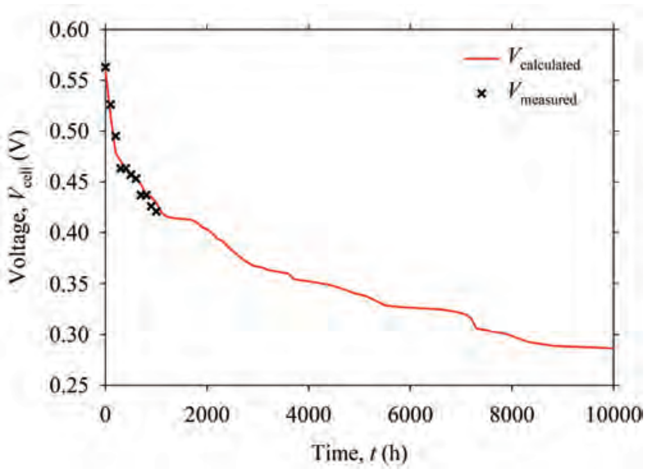

Figure 2: Calculated voltage ($V_{calculated}$) of solid-oxide fuel cell (SOFC) using the fitted model parameters based on the measured voltage ($V_{measured}$) at a current density of 0.45 A cm^{-2}.

In the area ***tools and building blocks for implementation*** most activities were carried out on the completion of three-year programme *Gostop - Building Blocks, tools and systems for factories of the future.* The work was carried out within the programme management, in the field of preparing a booklet with a presentation of the main achievements of the programme on its completion, as well as part of the R&D projects in which we participated in a number of R&D content areas. In the field of realization of product prototypes for smart factories of the future, we participated in further development, modifications and laboratory testing of modules to ensure 100% quality of a series of finished products in the case of a large number of lines for the production of various types of electric motors. In the field of the development of the platform for decision support and intelligent tool management, we participated in defining the requirements for the development of a larger number of technologies and modules and in testing the developed software tools. We have also prepared documentation for technical improvement, which formalizes the process for automatic identification of the production workflow from the event log. In the field of making the experimental concept of intelligent drive, we performed various experiments in order to determine the possibility of detecting faults on the drive from the vibration signal.

Applied research in the priority problem domains was the third 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 datasets preparation and the research of different Gaussian-process-based modelling methods for the identification of models useful for forecasting the short-term exposure to radiation. Datasets of atmospheric variables and computed virtual exposure to radiation were prepared and the selection of methods for identification in the project was pursued.

In 2020 we continued the work on the ARRS application project *Optimization based control of P2G converter connected to hydro power plant.* We received, refined and labelled the data from the partner HESS d.o.o. for the Brežice hydropower plant. The concept of a power-plant model was then designed in synergy with a power-to-gas system and other sustainable energy sources. It comprises models of physical components, such as generator, accumulation, electrolyser, hydrogen storage, solar cells, fuel cell, profiles of current data (electricity, river-flow, solar) and predictions of physical (weather, electricity, hydrogen) and economic (electricity prices, hydrogen prices, CAPEX, OPEX, etc.) parameters. Based on models from the literature and the data obtained, these were incorporated and tuned into coordinated models of the aforementioned subcomponents and combined into a working simulation model to form a whole. This now enables the development and implementation of an optimization control concept.

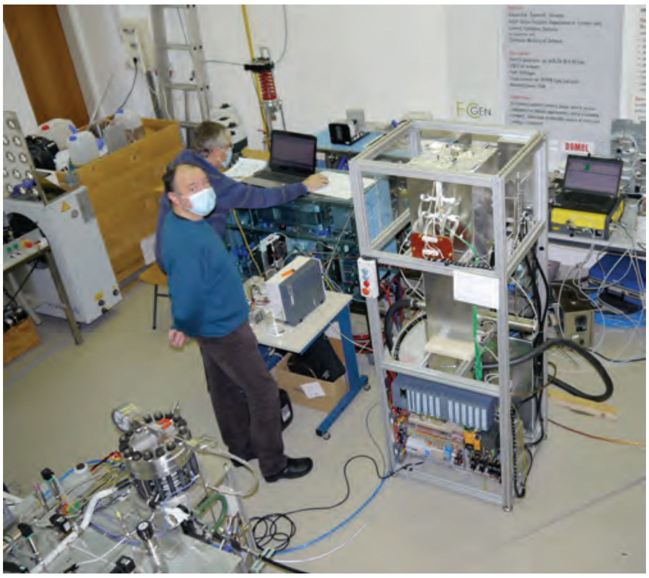

Figure 3: Closed-loop comparison of two-degrees-of-freedom PID controllers tuned with the developed tuning method.

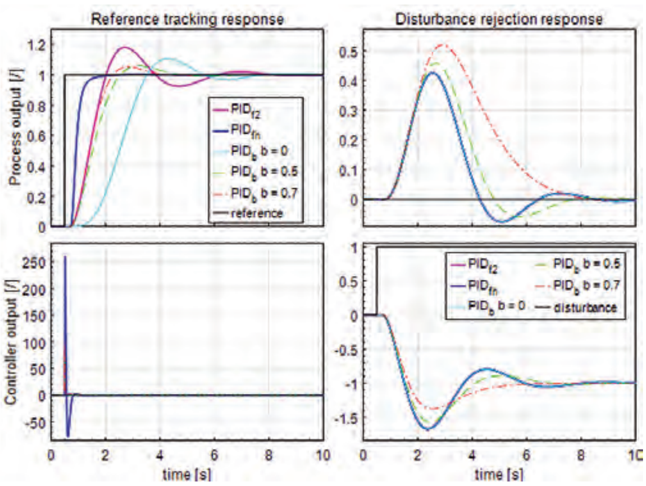

Figure 4: System IAPUNIT during commissioning

Integrating systems are common in various industries. Due to open-loop instability, efficient control of integrating systems remains a challenging task. In the research *"Parametric and Nonparametric PI/PID Controller Tuning Method for Integrating Processes Based on Magnitude Optimum"* we have developed a PI/PID tuning method for integrating processes based on Magnitude Optimum. The developed tuning method provides disturbance rejection or tracking-performance optimization with additional user-defined parameters, while the optimal overall closed-loop performance can be achieved with an additional reference filter (Figure 3).

Following the initiative of the Republic of Slovenia for the establishment and operation of Strategic Innovative Partnerships within the framework of the Slovenian Smart Specialisation Strategy S4, the *Strategic Innovative Partnership Factories of the Future - SRIP ToP* is also operating. Our department has a very active role in *SRIP ToP* in the management of the area *Control Technologies* and in the implementation of its Multi-Annual Action Plan. In 2020 we carried out all the envisaged activities of the Action Plan's second phase and prepared a detailed action plan for the third phase.

International R&D projects

In collaboration with *Technical University Graz* our team has pursued experimental research on health monitoring of solid-oxide cells, study of the relationship of the process parameters cell performance as well as strategies for safe and stable operation. Advancements have been achieved in the characterization of the cell condition by fast electrochemical impedance spectra, identification of the equivalent circuit model parameters from measured voltage and current in the time domain and change detection health condition based on changes in the spectra.

IAPUNIT is an international project partly financed by Slovenian *Ministry of Defence* in coordination with *European Defence Agency (EDA).* The project is from the field of hydrogen technologies and the main goal is the supply of military vehicles with the electrical energy generated by fuel cells powered by military diesel fuel with a high sulphur content. The

Department of Systems and Control and the National Institute of Chemistry Slovenia are developing a fuel processor (reformer) that converts military diesel into high-temperature-fuel-cell-grade hydrogen. In 2020 the system was finalized and tested successfully (Figure 4). Intensive coordination is under way with the European Defence Agency to continue the development to TRL 6.

In 2020 we continued research on the project *INEVITABLE - Optimization and performance improving in metal industry by digital technologies*, which has received funding from the the European Union's Horizon 2020 research and innovation programme. As project coordinator, we had more work due to COVID-19 crisis, as certain activities could not be performed due to closure of a partner's production and laboratory facilities. To be able to perform all the planned project activities, we have initiated procedures at the EC for a 6-month project extension. In addition to management and dissemination activities, the department is also responsible for carrying out the research tasks, with the main goal to digitalize the process of cold rolling of metal sheets at SIJ Acroni. Here, we are developing a supervisory system for a cold rolling machine, with which we will be able to monitor the production process and diagnose production equipment. During the implementation of this year's activities, we became familiar with the production process and the available data, we were participating in the modernization and digital upgrade of the production process and we set up a physical model framework of the machine. Together with the project partner Siemens, we also prepared technical validation of IoT and cloud solution that will be implemented into the SIJ Acroni's production process.

In 2020 we started carrying out work on the new research project "*HECAT - Disruptive Technologies Supporting Labour Market Decision Making*". HECAT is a Horizon 2020 funded research collaborative in the Societal Challenge 6 category (SC6) and comprises of research consortium, carefully brought together to achieve the task of developing an ethical-algorithmic-based platform to assist Public Employment Services (PES) and Unemployed people in making informed, transparent and integrated decisions. The research aims to use sociologically and anthropological insight into unemployment and the labour market to guide technical developers of the back-end algorithms and front-end user interface with the objective of creating an ethical and equal platform. The research is coordinated by the Waterford Institute of Technology and is supported by partners across Europe: Employment Service of Slovenia, University of Ljubljana, Copenhagen Business School, Platform Networking for Jobs, Roskilde University, Sciences Po, Jožef Stefan Institute and Tecnalia.

The second newly acquired project in 2020 under the Horizon 2020 program is the project *RUBY - Robust and reliable general management tool for performance and dUraBilitY improvement*. RUBY aims at developing and implementing a tool able to perform integrated monitoring, diagnostic, prognostic and control functions of solid-oxide and proton-exchange-membrane fuel cells. The JSI team has contributed novel results, the first such in the domain, which refer to the estimation of the fuel cells' model parameters along with their uncertainties. Hence, the random process noise and disturbances can be consistently considered, thus leading to more robust and reliable diagnosis.

Applied work

Feasibility study for HESS d.o.o. was carried out as part of the ARRS project entitled *Optimization based control of P2G converter connected to hydro power plant*, where we discuss the problem of optimal control of a special case of a system to convert electricity to hydrogen (P2G - Power to Gas System) connected to a hydroelectric plant. In the feasibility study we considered financial flows and stated in which cases and in what way it is economically viable for a hydropower plant to produce green hydrogen. We also proposed the three-phase implementation of the P2G system and defined the financial effects and the payback period of the investment.

Two diagnostic systems developed in the previous year for end-of-line quality control of electric bicycle drives (Pedelec) for Domel d.o.o. were upgraded in 2020 (Figure 5) to test several different drive types and to automatically detect the type and adapt the test procedure to it. As part of the upgrade, calibration procedures were improved and features were added to the system to test additional characteristics and parameters. Band-pass filters were tuned to detect rotor-balancing and crankshaft-bearing faults. Vibration signals at several operating points were recorded and stored for the future tuning of transmission-fault detection functions. In addition, a process-signal-recording algorithm was incorporated into the prototype system for the needs of developing an intelligent production control system.

Figure 5: Diagnostic System for End-Of-Line Quality Assessment of the Pedelec Electric Bike Drives

In the *KET4CP Micro Grant* project, mathematical modelling was used for the design of the reactor volume when upgrading a small wastewater treatment plant to an MBBR (moving-bed biofilm reactor) process with small, free-floating, plastic carriers with attached biomass. The innovation is a replacement of a part of plastics with an eco-friendly nanocellulose material. For the new type of carriers, we have adjusted the parameters of the MBBR mathematical model as well as tested the plant performance at different wastewater temperatures, carrier surface area, carrier filling fraction, different reactor configurations and long-term dynamic operation with weekly and seasonal input load variations.

At the end of 2020, we concluded an agreement with Domel d.o.o. on the development of a new diagnostic line for the end-of-line quality control of new types of electronically commutated electric motors. Compared to many diagnostic lines we have developed for Domel so far, the new device will be much more flexible and will enable the diagnosis of as many as four mechanically different types of motors (712, 720, 758, 759). Adaptation to the specific type will be completely automatic, in accordance with the principles of Industry 4.0 and the Factories of the future.

Educational and training activities

Some members of the department are giving lectures and practical courses at different faculties and universities: the Faculty of Electrical Engineering, University of Ljubljana, the Faculty of Logistics, University of Maribor, Faculty of Industrial Engineering Novo mesto, University of Nova Gorica and the "Jožef Stefan" International Postgraduate School.

Some outstanding publications in the past year

1. Nerat, Marko. A reduced-complexity model of the solid oxide fuel cell performance degradation due to the nickel agglomeration in the anode. *Journal of power sources*, ISSN 0378-7753, 2020, vol. 466, pp. 228309-1-228309-12, doi: 10.1016/j.jpowsour.2020.228309. [COBISS.SI-ID 16257795]
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Some outstanding achievements in the past year

1. The *Puh National Award for outstanding achievements* was awarded to dr. Janko Petrovčič from the Department of Systems and Control for the development of innovative electronic systems.
2. A member of the Department of Systems and Control, doc. dr. Damir Vrančić, was among the recipients of the *Award for the best innovations* of the *Chamber of Commerce and Industry of Osrednjeslovenska region* for 2020 for the innovation of smart drive's pressure controllers and valves for the field of district energetics.
3. Tadej Krivec, an associate of the Department of Systems and Management, was the recipient of the *Technology Network Technology Process Award* for the best master's thesis in 2020 entitled „Processing of complex events in monitoring the production process".
4. In 2020 the multi-annual program *GOSTOP - Building Blocks, Tools and Systems for the Factories of the Future* was successfully completed, where the Department of Systems and Control coordinated the *Control Technologies* program pillar and also participated in the coordination of the entire program.

Awards and Appointments

1. Tadej Krivec: received the PCT technology network award (Process Control Technology) for his master's thesis entitled "Complex event processing in production process monitoring", Ljubljana, Slovenia
2. Janko Petrovčič: received the highest national Puh Award for outstanding achievements for the development of innovative electronic systems. Ljubljana, Slovenia
3. Damir Vrančić: the silver award for innovation went to Danfoss Trata d.o.o. for Virtus iSET/iNET innovation of smart-operated pressure regulators and valves for district heating. A member of the awarded group was our department member. Chamber of Commerce and Industry of the central Slovenia region for the best innovations for 2020, Ljubljana, Slovenia

INTERNATIONAL PROJECTS

1. KET4CleanProduction Bor-plastika: Implementation of MBBR Technology
   Dr. Nadja Hvala
   Bor-plastika d. o. o.
2. IAPUNIT - Development of an Innovative Auxiliary Power UNIT for military purposes based on high-temperature PEM fuel cell and reforming technology for military logistic fuels
   Asst. Prof. Gregor Dolanc
   The European Defence Agency (eda)
3. H2020 - RUBY; Robust and Reliable General Management Tool for Performance and Durability Improvement of Fuel Cell Stationary Units
   Prof. Đani Juričić
   European Commission
4. H2020 - HECAT; Disruptive Technologies Supporting Labour Market Decision Making
   Asst. Prof. Pavle Boškoski
   European Commission
5. H2020 - INEVITABLE; Optimization and Performance Improving in Metal Industry by Digital Technologies
   Dr. Dejan Gradišar
   European Commission
6. 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. On-line Degradation Monitoring for Extended Durability of High Temperature Steam Electrolysers
   Prof. Đani Juričić
2. Degradation monitoring and performance optimisation of solid oxide electrolysis cells
   Prof. Đani Juričić
3. STRAP - Sources, TRansport and fate of persistent Air Pollutants in the environment of Slovenia
   Prof. Juš Kocijan
4. Method for the forecasting of local radiological pollution of atmosphere using Gaussian process models
   Prof. Juš Kocijan
5. Optimization based control of P2G converter connected to hydro power plant
   Asst. Prof. Gregor Dolanc
6. Stability of nuclear reactors in load follow mode of operation
   Dr. Boštjan Pregelj
7. Modelling the Dynamics of Short-Term Exposure to Radiation
   Prof. Juš Kocijan
8. 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
9. Building blocks, tools and systems for the Factories of the Future – GOSTOP
   Dr. Vladimir Jovan
   Ministry of Education, Science and Sport
10. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
    Asst. Prof. Gregor Dolanc
    Slovenian Research Agency

NEW CONTRACT

1. Modelling the Dynamics of Short-Term Exposure to Radiation
   Prof. Juš Kocijan
   Nuklearna Elektrarna Krško d. o. o.

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9. Prof. Đani Juričić
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11. Dr. Marko Nerat
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16. Dr. Darko Vrečko

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22. Žiga Stržinar, B. Sc.
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DEPARTMENT FOR ARTIFICIAL INTELLIGENCE E-3

Head:
Prof. Dunja Mladenić

The Department for Artificial Intelligence (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 Department for Artificial Intelligence 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; 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 the 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; 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 that allows a user to follow business and personal named entities in time and establish broad relations between named entities (based on shared Wikipedia concepts from news articles) as well as to view the changes in these relations, Graph Based Analytics (http://gba.ijs.si) a service for business relation identification from text that enables the identification of business relations, such as mergers&aquisitions, bankruptcy, earnings, dividends et al. 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/) and AIObservatory (https://infominer.ijs.si/). The department's strategy is to combine scientific excellence with strong industrial collaboration enabling the transfer of research results into real-world business environments.

Establishment of the International Research Centre for Artificial Intelligence (IRCAI) under the Auspices of UNESCO.

In October 2020 the "International Research Centre for Artificial Intelligence" was established in Slovenia under the auspices of UNESCO. The Minister of Education, Science and Sport, Dr. Jernej Pikalo, and the Deputy Director-General of UNESCO for Communication and Information, Dr. Moez Chakchouk, signed a formal agreement on the 5th of March 2020 on the establishment of the centre working under the auspices of UNESCO in Ljubljana.

In spring 2020 we set up the Corona Virus Media Watch tool, which tracks virus alerts in real time and also updates data on the global spread of the virus. In late July 2020 we co-organized the first virtual conference of the Eastern European region with the Ministry of Science, Education and Sports, Slovenian National Commission for

UNESCO and UNESCO. The consultation discussed the Recommendation for ethics in AI between experts and policy makers from participating countries. IRCAI and the French Institute in Slovenia jointly organized the AI-Please Mind the Gap event as part of the Digital November programme. The main question of the discussion was how to bridge geographical, socio-economic, gender and community gaps in AI. In late November 2020, we prepared a roundtable with the Slovenian National Commission for UNESCO entitled "Artificial Intelligence: Life in the Age of Robots and Transhumanism". In addition to organizing events, our staff participated as speakers in several events. In 2020 we started building the team and all the processes needed to run the centre. Care was taken to establish collaboration and appropriate communication with all stakeholders; academics, policy makers (all Slovenian embassies), industry and the general public. In addition to connecting with relevant networks dealing with IRCAI-specific topics, CAHAI confirmed observer status on IRCAI in December 2020.

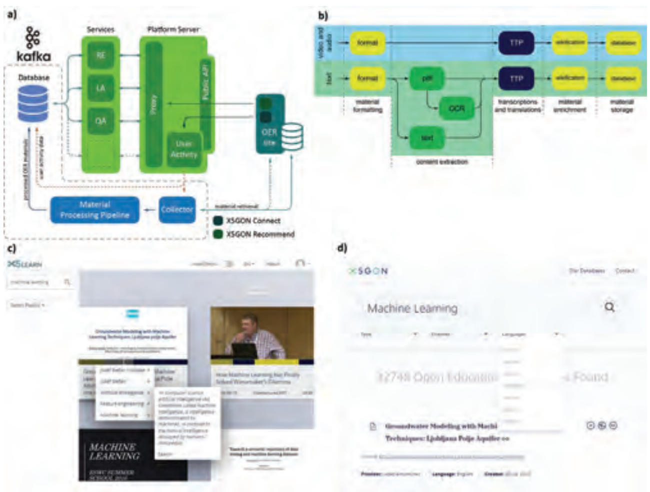

Figure 1: Architecture, pipeline and tools developed within the EU Horizon 2020 project x5GON: a) X5GON Platform Architecture, b) X5GON Processing Pipeline, c) X5Learn Interface, and d) the X5GON Discovery Tool.

The operation of the Centre has been structured in terms of programme committees, most of which are already assembled and working. The result of the work of the committees, in addition to strategic planning, is the launch of the IRCAI Award, which will support projects and solutions that, through artificial intelligence, make possible the achievement of the sustainable development goals as set by the United Nations.

For an efficient and optimized management of the workload and organization of business processes, we commissioned the development of the IRCAI website. In addition, intensive discussions began in 2020 with the publisher of scientific content, Cambridge University Press, with whom we intend to launch a new scientific journal that will be the first scientific publication of its kind, focusing on the Sustainable Development Goals and Artificial Intelligence.

Following the formal launch, IRCAI has started planning an event in March 2021, where the launch will be announced to all relevant stakeholders as well as the interested public through a press conference. Discussions and planning are also underway for the organization of a major event on digitalisation and artificial intelligence during the Slovenian Presidency of the Council of the EU.

Members of the Department of Artificial Intelligence have successfully continued participating in EU, national and regional projects. In the last 18 years the AILAB has participated in 77 EU projects, of which 6 were concluded in 2020 and 15 were still ongoing. The AILAB also participated in 9 national projects.

In 2020, in the area of **statistical data modelling and machine learning**, we successfully concluded four projects, **Perceptive Sentinel**, **enviroLens**, **TheyBuyForYou** and **DataBench** and are continuing work within **CogLo**, **Naiades** and **FACTLOG**. In the EU H2020 project **Perceptive Sentinel** (*BIG DATA knowledge extraction and re-creation platform*) an Eo-learn machine-learning framework that enables efficient data processing on the top of Big Data acquired from satellites within the Sentinel-1, -2 and -3 missions was successfully built. Numerous solutions have been developed for the efficient processing of data, among them: the FASTENER algorithm for an efficient feature-selection process for land-cover classification and rapids-ml library, which includes very fast implementation of stream mining algorithms. Both approaches have resulted in the speed-up of land-cover classification by an order of magnitude. The project successfully concluded in 2020. The EU H2020 project **enviroLENS** (*Copernicus for environmental law enforcement support*), which started in December 2018, concluded in December 2020. The aim of the project was to assist personnel involved in environmental legal issues (legal firms, non-government organization, etc.). This support includes identifying environmental changes, as well as providing relevant legal documents associated with the provided area and environmental issues. This was achieved with the usage of methods in the remote-sensing/earth-observation (EO) domain combined with natural language processing. All these methods are integrated into the eLENS Portal – a portal which enables the user to monitor environmental changes associated with a topic (e.g., deforestation) in the selected area and receive notifications regarding these changes. The Department of Artificial Intelligence developed the eLENS Miner System, which enables the user to search for relevant legal documents associated with a given environmental topic and geographical area. The system is able to, 1) process new legal documents, 2) search for relevant legal documents, and 3) search for similar legal documents given another legal document. The system and its documentation are available at http://envirolens.ijs.si/. In the last year of the project, we have evaluated the models with our project partners, identified possible problems and provided solutions, resulting in the successful completion of the project. The fourth EU H2020 project that concluded in 2020 is **DataBench** (*Evidence Based Big Data Benchmarking to Improve Business Performance*), within which the Department for Artificial Intelligence developed the *DataBench Index* and *DataBench Observatory tool*. This is a tool for observing the popularity, importance and the visibility of topic terms related to Artificial

Intelligence and Big Data, with particular attention dedicated to the concepts, methods, tools and technologies in the area of Benchmarking. The *DataBench Observatory* introduces the popularity index, calculated for ranking the topic terms in time, which is based on the following components: (i) Research component, such as articles from the Microsoft Academic Graph (MAG); (ii) Industry component, such as job advertisements from Adzuna service; (iii) Research and Development component, such as EU research projects, e.g., in CORDIS dataset (iv) Media component, such as cross-lingual news data from the *Event Registry* system; (v) Technical Development component, such as projects on Github; and, (vi) General Interest, such as Google Trends. The *DataBench Observatory tool* has been integrated into the *DataBench Toolbox* and presented at consortium meetings and external dissemination events. 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 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, a methodology for optimization of resources on graph distribution, and a methodology for large graph processing with clustering. Algorithms for an assessment of logistics events in real time enable an assessment of optimal response to the ad-hoc requests for interventions in logistics parcels delivery. The analytical pipeline was integrated and tested in a demo solution. The integrated solution was presented and implemented on real-case scenarios in three different test-bed sites, namely: Slovenia-Croatia (the cross-border region from Brežice to Zagreb), Greece (Athens) and the Logistic chain of EKOL with a pilot from Italy (Trieste) to East Europe (Poland). In the scope of the project, a *Cognitive Adviser Tool* was developed as a main agent monitoring events in the infrastructure in real-time and creating interventions for 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 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 water supply for a given settlement and apply predictive models, that would help get additional insights into their future changes. In 2020 we have conceptualized and delivered all of the core components upon which AI services will be built. We have identified and tested data sources, data models as well as underlying architectures for the technical solutions. We have also delivered all of the key components for the final solutions. In coordination with the Naiades consortium, one of our tasks has been 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 the 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. In the project, the Department for Artificial Intelligence is leading the development of analytical tools. Together with partners, we have designed a framework in which the machine-learning models work together with domain expert models and optimisation algorithms to solve industry problems. The implemented methods are tested in several different business cases. We support two of them: JEMS, a Slovenian company processing waste into fuel and Tüpraş, a Turkish oil refinery.

We have successfully concluded six EU H2020 projects: DataBench (Evidence Based Big Data Benchmarking to Improve Business Performance), TheyBuyForYou (Enabling procurement data value chains for economic development, demand management, competitive markets and vendor intelligence).

In the area of **data-streams analysis**, we continued the development of the *Platform for Anti Money Laundering* and *Counter Financing of Terrorism* as one of the 15 fin-tech 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*). In close cooperation with the Bank of Slovenia, which is a partner in the project, we have developed the *Risk Assessment tool*, which is already installed at their site. During activities of data discovery and data gathering, we faced unforeseen challenges regarding data privacy, which are being resolved. Our second project in this area is the EU project **CyberSANE** (*Cyber Security Incident Handling, Warning and Response System for the European Critical Infrastructures*), which 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. In 2020, we started working with partners to develop technology to capture and analyse structured and unstructured data from the so-called dark web as well as from media articles. 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.

In the areas of **text and network analysis and language technologies**, we are part of the EU H2020 project **SILKNOW** (*Silk heritage in the Knowledge Society: from punched cards to big data, deep learning and visual / tangible simulations*). Within the project we have developed methods for multilingual text annotation based on our Wikifier service, extending it with terms from the SILKNOW thesaurus http://wikifier.org/silknow.html. The service was successfully applied on real-world data from the museums to enrich the *SILKNOW Knowledge Graph*. We have developed a semi-automatic approach to investigate the relationship between the SILKNOW thesaurus and the existing Getty thesaurus. We have developed an approach to information extraction from textual descriptions of the museums and validated it with domain experts on English, French and Spanish texts. We have continued our coordination of the EU Horizon 2020 project **ELEXIS** (*European Lexicographic Infrastructure*) which 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 2020, in addition to the activities related to project management, we have been maintaining the project website, updating the contents and functionality of the Elexifinder tool. We have also launched the crowdsourcing mobile app *Game of Words*, available for Android and iOS devices. We have continued improving and testing the *Elexifier conversion tool*; over 200 dictionaries have now been converted with the tool and included in the database. We have also continued with the development of the Lexonomy dictionary writing system. In particular, we have worked on the widget, improving user experience when using the Sketch Engine API, and developed the manual linking feature, which will be part of the Dictionary Matrix ecosystem and will be used for creating, viewing and editing links between dictionaries. Based on agreements with partner and observer institutions, we have obtained over 80 different lexical resources, covering over 20 different languages and containing over 30 million entries. More than 50 of those resources have been uploaded to Lexonomy for linking purposes. Within the H2020 EU Marie Skłodowska-Curie ITN project ***CLEOPATRA*** (*Cross-lingual Event-centric Open Analytics Research Academy*), two Early-Stage Researchers were employed full-time by our department and began work on the topics "*Information propagation with barriers*" and "*Cross-lingual news reporting bias*". Both presented their first results at SiKDD 2020 - Conference on Data Mining and Data Warehouses, organized within Information Society Multiconference. In 2020, *CLEOPATRA* organized the "First R&D Week" including Hackathon, the "Second Learning Week" and the "Second Hackathon CKPP and Demonstrator session". All of the events in 2020 were held virtually, which in some cases ensured that a wider international audience was reached than would have been the case for a face-to-face workshop or conference.

x5Gon (Cross Modal, Cross Cultural, Cross Lingual, Cross Domain, and Cross Site Global OER Network) EnviroLENS (Copernicus for environmental law enforcement support), PerceptiveSentinel (BIG DATA knowledge extraction and re-creation platform) and Humane AI (Toward AI Systems That Augment and Empower Humans by Understanding Us, our Society and the World Around Us)

The area of **text and network analysis and language technologies** has also included work in national and regional projects. In 2020, we have also started working on the project ***Development of Slovene in a Digital Environment*** (Slovene: Razvoj slovenščine v digitalnem okolju, RSDO). It 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. Its outcomes include new language resources, tools and applications for processing Slovene (upgraded corpora, speech recognition, semantic technologies, machine translation, a terminology portal, and language technology center maintenance - CLARIN.SI). In the first year of the project, we have begun coordinating student work for the annotation of the Sloleks lexicon and the ssj500k corpus. Furthermore, we have begun developing the MultiCOMET tool. MultiCOMET is a commonsense knowledge model which can generate context statements from an input sentence. This includes conditions and consequences of the event in the input. A deep neural network model parses the input and infers the facts regarding its circumstances and effects. In December 2020 we presented the project at the online event MetaForum 2020. In 2020, we finished coordinating the ARRS project ***New grammar of contemporary standard Slovene: sources and methods***, which began in 2017. The project aimed to explore linguistic methodological foundations of a complex analysis of written and spoken Slovene, as found in the new corpora developed in recent projects. The resulting methodology and data will provide a sound foundation for future work on an empirically based description of Slovene. Following from the methodology, we compiled and published extensive collections of extracted material from corpora that will be useful for the development of language-technology applications for Slovene. The extracted data will be used for the linguistic analysis of real language, which represents the first step towards the compilation of a new descriptive corpus grammar of Slovene. In line with these goals, in the last year, we participated in the design and development of several tools for lexical data extraction from text corpora (morphology, wordlists, collocations, multi-word expressions, n-grams), and their related analysis. We have published a collection of lists with linguistic data from Slovene reference corpora (Gigafida) and spoken corpora (GOS). The lists contain different levels, from individual symbols in words to n-grams. They were prepared using the program LIST, which was developed in this project and can be used to create similar exports from other corpora databases. The guide to the frequency lists is available at: https://e-knjige.ff.uni-lj.si/znanstvena-zalozba/catalog/book/250. We were also part of the ARRS project ***Collocations as a Basis for Language Description: Semantic and Temporal Perspectives***, whose main objective is to conduct basic research into semantic and temporal aspects of collocation, as well as statistics for measuring it, areas that have been so far largely neglected in Slovenian linguistics, and to some extent also internationally. In 2020 the department took part in analysing how collocation trends change through time. The analysis will be presented in the project monograph. Results also include a tool for tracking changes in the Slovene language. The overall objective of the Multilingual Resources CEF project **MARCELL** is to provide automatic near-translations on the body of national legislation (laws, decrees, regulations) in seven countries: Bulgaria, Croatia, Hungary, Poland, Romania, Slovakia and Slovenia. At present, national legislation texts are not automatically available to CEF.AT and current Machine-Translation (MT) systems could be improved if they had access to national legislative texts, enriched with metadata (lemmatization, linguistic annotations, IATE terminology and EUROVOC descriptors. In 2020 our activities were focused on semantic micro-alignment (https://marcell-alignment.ijs.si) as well as improvements to corpora annotation and document classification algorithms. Together with the Department of Knowledge Technologies (E8), we continued to lead the Slovene research infrastructure **CLARIN.SI**, which provides easy publication and sustainable access to digital language data for scholars in the humanities and social sciences. In addition to providing support for the CLARIN.SI repository, we also contributed various types of data (lexical resources, corpora, training corpora) and technologies (grammatical annotation, lexical data mining) for Slovene language processing.

In the area of **semantic technologies**, we have completed the EU Horizon 2020 project **TheyBuyForYou** (*Enabling procurement data value chains for economic development, demand management, competitive markets and vendor intelligence*). As part of the project activities, we have developed a Knowledge Graph containing data on public procurement in many European countries. It is freely accessible and compatible with Open Contracting Standard. As part of the project, our team developed an online platform to analyse public procurement and spending. In the process, we collaborated with the Ministry of Public Administration, which aims to ensure transparency in the use of public funds and prevent corruption and other irregularities in the use of public funds. Our platform accessible at http://tbfy.ijs.si, enables the detection and visualization of anomalies in public procurement and financial transactions. In the national project **Causalify**, we have developed a theoretical framework for modelling dynamic graphs of interrelated events as a hierarchical multi-layered complex system. Based on this, we have developed an approach to modelling social dynamics which we have validated on the problem of monitoring dynamics in a society based on a selected sample of news. The developed model was adjusted in two ways to handle two related problems: monitoring user mobility and predicting development of science in the sense of predicting popular research topics.

Figure 2: Top: Establishment of the International Research Centre for Artificial Intelligence (IRCAI) under the Auspices of UNESCO. Bottom: The Corona Virus Media Watch European dashboard that uses global and national news updates to create powerful narratives and visualizations, that ultimately can take us further into future predictions of how the pandemic is evolving across the world. The image shows a snapshot of the 5D Visualization on March 23rd. Countries that were at the peak in terms of growth are shown high (for example, Turkey), whereas countries that mostly contained the virus are shown lower down (for example, China).

In the area of **knowledge management**, the group's focus includes research and development by using methods and tools from a broader artificial intelligence area in real business settings. We have successfully concluded the EU H2020 project **X5GON** (*Cross Modal, Cross Cultural, Cross Lingual, Cross Domain, and Cross Site Global OER Network*) in December 2020. The goal of the projects was to implement innovative technology elements for connecting the scattered Open Educational Resources (OER) available across Europe and the globe, as well as to improve the learning experience of all within the education domain, e.g., students, teachers, researchers, resource providers and decision makers. To achieve these goals, we developed several services, that: 1) are able to process text, video and audio files, translate them into seven languages, and enrich them with annotations, 2) provide personalized recommendations of resources based on the users past viewing, and 3) enable quick search through the OERs with the possibility of filtering them by license, resource type and language. These services are used within various products, which were extended with additional methods and functionalities. Among them are the *X5GON Discovery Tool* (https://discovery.x5gon.org/), the learning environment for the blind and visually impaired *X5GON*

Blind (https://blind.x5gon.org/), the educational environment *X5Learn* (https://x5learn.org/), the learning analytics machine (https://analytics.x5gon.org/), as well as plugins for providing resource recommendations and integration into the learning environment Moodle. All of these products are public and available on the *X5GON Platform* (https://platform.x5gon.org/). In addition, the platform enables the user to access the processed resource metadata via the open API. In 2020 we continued with the **Water4Cities** (*Integrated Surface and Groundwater Management for Sustainable Urban Development*) project under the EU Horizon 2020 Marie Skłodowska Curie RISE project together with Centre for Knowledge Transfer in IT. We continued with data analysis on groundwater, rivers and stormwater flow data in the Ljubljana aquafier and water quality and consumption in the Greek island of Skiathos. We continued with development of models and a platform that will allow us to monitor optimal water management in real time. In 2020 we published regular webinars, which are available on the 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 leading European research centres, universities and industrial enterprises into a network of Centres of Excellence. Leading global Artificial Intelligence (AI) laboratories will collaborate with key players in areas, such as human-computer interaction, cognitive, social and complexity sciences. The project is looking forward to drive researchers out of their narrowly focused field and connect them with 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 goal of the EU Horizon 2020 project **FIN-TECH** *(A FINancial supervision and TECHnology compliance training programme)* is to develop a program for the exchange of knowledge in the financial environment. In this manner, the goal of the FINTECH project is to create a European training programme, aimed at providing shared risk management solutions that automatize compliance of Fintech companies and, at the same time, increase the efficiency of supervisory activities. The project incorporates 24 partners covering all 28 European countries, plus Switzerland. Within this project, our department collaborates with the Bank of Slovenia in order to provide insight and knowledge in the technical aspects of this rapidly developing field. In 2020 we prepared an online workshop on Artificial Intelligence. 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 a prototype of the automatic web-based tool, which will allow evaluation of textbooks based on their textual and pictorial properties. The tool will support decision-making process for selection of appropriate textbook. In 2020 we developed a tool for scoring text readability in Slovene. It is available at: https://orodja.cjvt.si/berljivost/.

Promotion of science is continually present in the efforts of our Department. In 2020, members of the Department for Artificial Intelligence were very active in promoting Artificial Intelligence and science in general.:

- Marko Grobelnik gave over 10 interviews on various media speaking about topics such as: Corona Virus Media Watch, IRCAI centre, AI and various EU projects
- Dunja Mladenić participating on a panel entitled: "The Mis-portrayal of AI in the Media: What to do about it?"
- Marko Grobelnik was a panellist at Bled Strategic Forum 2020
- Marko Grobelnik was a panellist on WSIS forum 2020
- Aljaž Košmerlj was a panellist at a roundtable entitled: "Coexist with AI – Vision of the Society 5.0"

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 2020, 168 students from 26 schools participated in the competition. We have also been active in promoting women in science offering 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 related international news (http://ScienceWithArt.ijs.si/).

In 2020 we were very actively involved in submitting new project proposals, particularly within the EU Horizon 2020 Programme. Once again, we were very successful, obtaining funding for three new projects: ***STAR, EUJapanAI*** and ***ODEUROPA***. We continue with our successful efforts to include the Slovenian industry into the European research area, where over the last 18 years we have contributed to a list of numerous companies participating in EU projects.

Some outstanding publications in the past year

1. Pérez, Manolo, Mladenić, Dunja, et al. From historical silk fabrics to their interactive virtual representation and 3D printing. *Sustainability*. 2020, vol. 12, no. 18, str. 7539-1-7539-22.

2. Koprivec, Filip, Kenda, Klemen, Šircelj, Beno. FASTENER feature selection for Inference from Earth observation data. Entropy. 2020, vol. 22, no.11, pp. 1198-1-1198-27
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4. Taherizadeh, Salman, Grobelnik, Marko. Key influencing factors of the Kubernetes auto-scaler for computing-intensive microservice-native cloud-based applications. Advances in engineering software. [Print ed.]. 2020, vol. 140, pp. 102734-1-102734-11
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Organization of Conferences, Congresses and Meetings

1. H2020 Theybuyforyou project meeting, Ljubljana, Slovenia, 28–29 January 2020
2. FIN-TECH AI worskhop: Uporaba AI v finančnem sektorju – praktični primeri, Ljubljana, Slovenia, 6 April 2020
3. CLASSLA K Centre workshop, Ljubljana, Slovenia, 6–8 May 2020 (virtual)
4. Spletno posvetovanje : Priporočila o etiki umetne inteligence, Ljubljana, Slovenia, 27–29 July 2020 (virtual)
5. Conference "Jezikovne tehnologije in digitalna humanistika", Ljubljana, Slovenia, 24–25 September 2020 (virtual)
6. Webinar AI-Please Mind the Gap, Ljubljana, Slovenia, 17 November 2020 (virtual); *co-organised together with The French Institute of Slovenia*
7. Round Table "Umetna inteligenca: Življenje v času robotov in transhumanizma", Ljubljana, Slovenia, 19 November 2020 (virtual); *co-organised with Slovenian National Commission for UNESCO*

INTERNATIONAL PROJECTS

1. European Language Grid (GA 825627)
   Asst. Prof. Simon Krek
   Dfki Gmbh - Deutsches Forschungszentrum Fuer
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. COST CA16105; European Network for Combining Language Learning with Crowdsourcing Techniques
   Asst. Prof. Simon Krek
   Cost Office
6. COST CA18209; European Network for Web-Centred Linguistic Data Science
   Asst. Prof. Simon Krek
   Cost Association Aisbl
7. COST CA18231; Multi3Generation: Multi-Task, Multilingual, Multi-Modal Language Generation
   Marko Grobelnik
   Cost Association Aisbl
8. H2020 - Water4Cities; Holistic Surface Water and Groundwater Management for Sustainable Cities
   Marko Grobelnik
   European Commission
9. H2020 - X5gon; Cross Modal, Cross Cultural, Cross Lingual, Cross Domain, and Cross Site Global OER Network
   Marko Grobelnik
   European Commission
10. H2020 - PerceptiveSentinel; BIG DATA Knowledge Extraction and Re-creation Platform
    Prof. Dunja Mladenić
    European Commission
11. H2020 - DataBench; Evidence Based Big Data Benchmarking to Improve Business Performance
    Marko Grobelnik
    European Commission
12. H2020 - TheyBuyForYou; Enabling Procurement Data Value Chains for Economic Development, Demand Management, Competitive Markets and Vendor Intelligence
    Marko Grobelnik
    European Commission
13. 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
14. H2020 - COG-LO; COGnitive Logistics Operations through secure dynamic and ad-hoc collaborative networks
    Marko Grobelnik
    European Commission
15. H2020 - EnviroLENS; Coprenicus for Environmental Law Enforcement Support
    Marko Grobelnik
    European Commission
16. H2020 - Cleopatra; Cross-Lingual Event-Centric Open Analytics Research Academy
    Marko Grobelnik
    European Commission
17. H2020 - Humane AI; Toward AI Systems That Augment and Empower Humas by Understanding Us, our Society and the World Around Us
    Marko Grobelnik
    European Commission
18. H2020 - FIN-TECH; A FINancial supervision and TECHnology compliance training programme
    Marko Grobelnik
    European Commission
19. H2020 - NAIADES; A Holistic Water Ecosystem for Digitisation of Urban Water Sector

Marko Grobelnik
European Commission
20. H2020 - CyberSANE; Cyber Security Incident Handling, Warning and Response System for the European Critical Infrastructures
Marko Grobelnik
European Commission,the Directorate-general
21. 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
22. H2020 - FACTLOG; Energy-aware Factory Analytics for Precess Industries
Prof. Dunja Mladenić
European Commission
23. H2020 - HumanE-AI-Net; HumanE AI Network
Marko Grobelnik
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. Collocation as a basis for language description: semantic and temporal perspectives
Asst. Prof. Simon Krek
2. New modes and Global Patterns of Online News (Re)production
Prof. Dunja Mladenić
3. New grammar of modern standard Slovene: resources and methods
Asst. Prof. Simon Krek
4. Causalify - Causality in global social dynamics
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. Preparation and Analysis of Data for Workshops
Dr. Iztok Kosem
Universidade De Coimbra
9. CLARIN Project: The CLASSLA Workshop on Using Language Resources and Tools for South Slavic Languages in Linguistic Research
Asst. Prof. Simon Krek
Clarin Eric

VISITOR FROM ABROAD

1. Marko Tadić, University of Zagreb, Faculty of Humanities and Social Sciences, 8 February 2020

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17. Manolo Pérez *et al.* (16 authors), "From historical silk fabrics to their interactive virtual representation and 3D printing", *Sustainability*, 2020, **12**, 18, 7539.
18. Vasja Vehovar, Blaž Povž, Darja Fišer, Nikola Ljubešić, Ajda Šulc, Dejan Jontes, "Družbeno nesprejemljivi diskurz na Facebookovih straneh novičarskih portalov", *Teorija in praksa: revija za družbena vprašanja*, 2020, **57**, 2, 622-645, 694.

Published Conference Contribution

1. Dejan Štepec, Tomaž Martinčič, Fabrice Klein, Daniel Vladušič, João Pita Costa, "Machine learning based system for vessel turnaround time prediction", In: *MDM 2020, 21st IEEE International Conference on Mobile Data Management, Versailles, France, 30 June-3 July 2020*, Proceedings, IEEE, 2020, 258-263.
2. Nikola Ljubešić, Ilia Markov, Darja Fišer, Walter Daelemans, "The LiLaH emotion lexicon of Croatian, Dutch and Slovene", In: *PEOPLES 2020, Computational Modeling of PEople's Opinions, PersonaLity, and Emotions in Social media, Barcelona, Spain, December 12-13, 2020*, Proceedings, (ACL Anthology), Association for Computational Linguistics, 2020, 153-157.
3. Jingbo Yang, Ruge Zhao, Meixian Zhu, David Hallac, Jaka Sodnik, Jurij Leskovec, "Driver2vec: driver identification from automotive data", In: *6th Workshop on Mining and Learning from Time Series, Aug. 24th, 2020, San Diego, California, USA*, Proceedings, 2020.
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2. Bowen Liu, *Machine learning for small molecule lead optimization:* doctoral dissertation, Stanford, 2020 (mentor Jurij Leskovec).
3. Emma Pierson, *Data science for social equality:* doctoral dissertation, Stanford, 2020 (mentor Jurij Leskovec).

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 increased trustworthiness of information and communication technologies and services.

Head:
Asst. Prof. Tomaž Klobučar

The research in 2020 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 in the EU Horizon 2020 projects "CONCORDIA", "Defender", "Compact", "DE4A", "BD4OPEM" and "iFlex", the EU DG Justice "EIO-LAPD" project, the "SI-PASS 2.0" project from the CEF programme, the national "Technological and business aspects of future ecosystem for e-health" project, and an industrial project "Use Wisely" with Elektro Celje. The focus was on the development of technologies and services in advanced next-generation networks, security and privacy in information systems, and technology-enhanced learning.

Members of the laboratory are teaching at the undergraduate and graduate levels at the Jožef Stefan International Postgraduate School, the DOBA Faculty, and Faculty of Commercial and Business Sciences. The laboratory is a member of European Cyber Security Organisation (ECSO).

Concepts and architectures of the secure internet, internet technologies and information systems

The first area of research and development was focused on 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 is to set up secure cross-border services, based on national electronic identification means, in different application domains. The SI-PASS 2.0 project, which is coordinated by the Laboratory for Open Systems and Networks, has 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 one hand, it connects the national infrastructure with foreign service providers and, on the other, the national identity and service providers with the infrastructures of other EU countries. The results of the project enable citizens of the 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 will simplify the cross-border user's interaction with the selected procedures, systems and platforms, and demonstrate in practice the benefits for different stakeholders of realizing across borders the principles of Once-Only and Digital-by-Default. Our main role in the project is to coordinate the Studying Abroad pilot, one of the three project pilots. The pilot will implement and validate the cross-border higher-education procedures of Single Digital Gateway Regulation, in particular applications to higher-education institutions, applications for study grants, and recognition of diplomas. In 2020 we defined the pilot's use cases in detail, identified their requirements, and prepared a solution architecture for the pilot. An assessment of existing building blocks and infrastructures, such as the eIDAS infrastructure, European Digital Credentials infrastructure, or European Blockchain Services infrastructure, was also conducted to investigate which building blocks can be reused by DE4A services and infrastructure. 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 **Defender** ("Defending the European Energy Infrastructures") project was addressing the issues of European critical energy infrastructures' security and dependability. A three-year project aimed at improving the protection of all energy domain segments, from generation, transmission to distribution. The improvements result in better infrastructure resilience and dependability. The project was the only large-scale project funded through the Horizon 2020 mechanisms that addressed the critical energy infrastructure protection. Besides a number of excellent European industrial partners, it had a strong Slovenian consortium, namely, the Laboratory for Open Systems and Networks together with Department of Communication Systems at Jožef Stefan Institute, Slovenian transmission operator ELES and Institute for Corporative Security Studies (ICS). The laboratory led work on cyber-physical threat assessment and analysis, led piloting and evaluation, and contributed to the development and implementation of the project's threat-mitigation and situational awareness solutions. In 2020 we led the final project solutions evaluation in Italy and Slovenia. In southern Italy we tested protection mechanisms against drone attacks and against attacks by armed terrorist forces on large distributed photovoltaic power plants. In the distribution network near Rome, we tested protection against cascading threats – water and energy infrastructure – and the detection and localisation of failures in the distribution grid. In Slovenia, the laboratory supported the evaluation in the ELES transmission network in Okroglo, a switching station near Kranj. During the piloting we measured the impact of weather conditions on the optical network in ground wires of transmission lines in the Primorska region and evaluated ways to model the state of the electrical network based on the conditions of the optical lines. In Okroglo we evaluated the mechanisms of protection against combined cyber-physical attack on the switching station and nearby electricity lines. We also evaluated the options of drone-based predictive maintenance of the switching field, transformers, poles, and power lines. The project was successfully completed in late 2020.

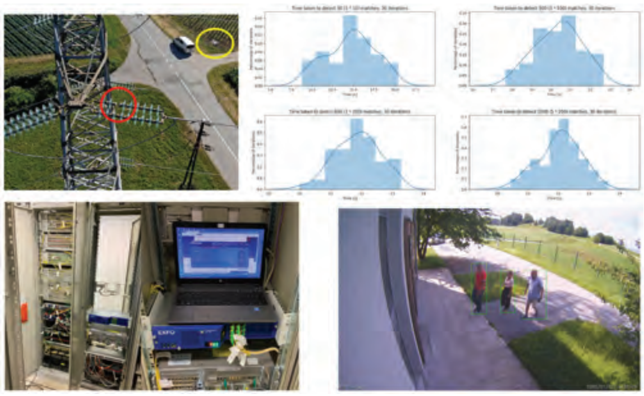

Figure 1: Threat detection in critical infrastructure

At the end of 2020 the **Use wisely** project started. The project aims at evaluating flexibility services in a distribution network. The laboratory project work focuses on data analytics, peak forecasting, consumer response assessment, and cloud services support. In the project, we will evaluate the end users' response to positive tariffs and their ability to lower critical peaks and the response to negative tariffs and the end users' ability to consume more energy during a surplus of photovoltaic generation. In 2021 a large-scale test of positive and negative critical peak tariff with more than 800 consumers will be conducted in the Celje region. Other partners in the project, which is financed by the Agency for Energy, are Elektro Celje, Smart Com and Comsensus. The Agency has also approved grants for the use of positive and negative tariffs in 2021.

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. In 2020, we led the collection and analysis of use cases related to the marketplace and potential energy services to be developed in the project. Two JSI departments, our laboratory and the Department of Communication Systems, participate in the project, while a key Slovenian partner from the energy sector is Elektro Celje.

The **iFlex** ("Intelligent Assistants for Flexibility Management") project focuses on the design, development and evaluation of supporting tools for consumers' successful participation in various flexibility services of the smart grid of the future and for their easier pursuit of sustainability goals in their premises. The project started at the end of 2020 and is funded by the Horizon 2020 programme. A strong Slovenian consortium is participating in the project: Elektro Celje, Elektro Celje Energija, Smart Com, Slovene Consumers Associations, and the JSI's Laboratory for open systems and networks. The tasks of the laboratory include security and privacy of the project solution, data analytics, consumer profiling, and development of a digital twin of the consumer premises.

The infrastructure programme services proved crucial to the smooth operation of the Institute during the COVID-19 pandemic.

In addition to the energy sector, another focus of our R&D activities was on e-health. The research project titled "**Technological and business aspects of future ecosystem for e-health**" aimed at implementing the work within the priority area of the European cohesion policy "Smart cities and communities". Its basic objective was to create a functional model to ensure sustainable technological and business development of an ecosystem for e-health. We were presented with a case study of the Slovenian healthcare ecosystem, and discussed our preliminary list of success factors for the maturation of a successful healthcare ecosystem. Our findings underlined the importance of the ecosystem's community and its strong role in the growth of a national ecosystem. The entire e-healthcare system needs to be protected from every type of threat at all times, from sensors and the Internet of Things to the core network and everything in between. Therefore, we have addressed the challenges of security and privacy of healthcare data, and the implications for interoperability in the e-healthcare environment. Understanding these challenges is critical for anyone working in healthcare.

As part of the Infrastructure program in research organizations we continue to provide support services that enable better communication among members of the various research programs, as well as students and their mentors from geographically dispersed institutions. The services proved crucial to the smooth operation of the Institute during the COVID-19 pandemic. With the help of research infrastructure services, more than 2,500 meetings were held at JSI in 2020 with 13,000 participants for a total of 7,500 hours (312 days), and we supported 31 departments, laboratories, centres and other organizational units of the Institute. We also supported the organization and implementation of Science Festival 2020 and Researchers' Night 2020.

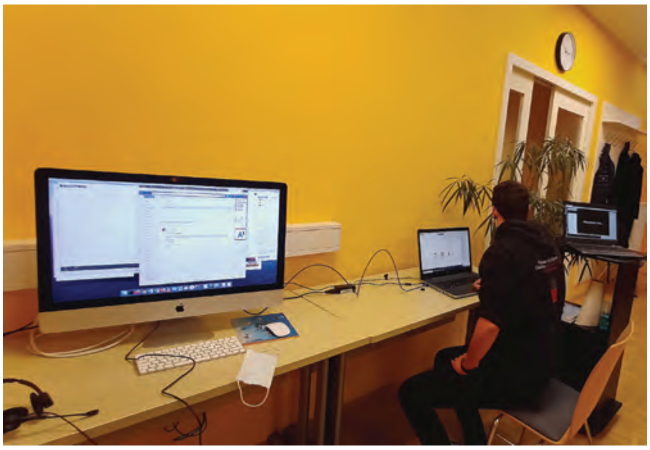

Figure 2: Support services of the infrastructure programme for the organisation of online conferences

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 2020 the researchers of the Laboratory worked intensively on developing solutions and systems for the provision of the necessary security mechanisms.

Our research and development results enable a more secure information society.

In this context, vulnerabilities and potential intrusions into communication privacy on the mobile Internet were identified, and a model specifying the main factors influencing the phenomena threatening user privacy was developed. In addition, a new method and software tool were developed 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 have been 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 tool is suitable for personal use by web system owners who can regularly check their servers and updated applications for vulnerabilities. This service is available to users at home and around the world. We have conducted a comparative analysis of the vulnerabilities on WordPress websites between thirty European countries.

Another research topic was mathematical models for constructing significant Boolean functions used in symmetric cryptographic algorithms. Except for small values, there is no classification of bent Boolean functions under the action of the general affine group, and the structure of the set of bent Boolean functions is not clear. When a new construction method is found, in order to show that it does not only yield functions that can be obtained by already-known methods, it is necessary to prove that some constructed functions are affinely inequivalent to Maiorana–McFarland functions (checking this with this class is usually considered obligatory because this class is simpler and provides the widest class of bent functions). For a cubic bent functions, therefore, the necessary and sufficient conditions concerning affine equivalence have been identified. While the design and properties of bent Boolean functions have been frequently addressed during the last decades, there are only a few design methods of so-called 5-valued spectra Boolean functions whose Walsh spectra takes only five values. In this direction, we have also proposed several classes of 5-valued spectra Boolean functions.

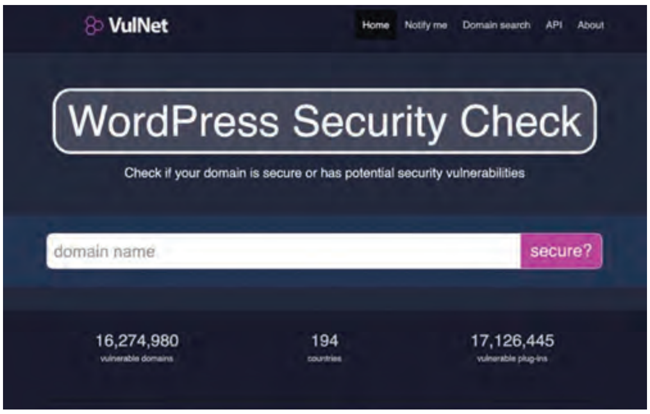

Figure 3: A tool for identifying vulnerable websites on a large scale

The growth of ubiquitous and pervasive computing systems with complex, heterogeneous, dynamic and mobile components, makes the use of structured overlay networks more desirable because of their inherent flexibility and extensibility to support modern applications. However, the performance and dependability of structured overlay networks depend on their fault tolerance and self-managing capability to ensure an acceptable level of service in the face of mobility and anticipated churn. In 2020, we provided a taxonomic analysis of existing churn-handling mechanisms and their qualitative comparison along with a detailed description of the factors behind the churn behaviour of the overlay participants in the existing applications. We also highlighted key research issues to guide future research in churn handling.

Research on the acquisition of cross-border digital evidence in crime investigation, enabled by the implementation of Directive 2014/41/EU and Slovenian legislation, continued in 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 institutions from Austria, Croatia, Italy, Germany and Portugal. In 2020 the current challenges and problems in providing cross-border digital evidence in criminal investigations were explored and appropriate technological and legal solutions to remove existing barriers within the European justice were proposed.

Figure 4: Virtual-reality-based active participation at an online conference

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 contributes with 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 and is also contributing with data and models for developing threat intelligence models, as well as with cybersecurity education activities. In 2020 the Laboratory was also involved in the Women in cybersecurity activities, contributing to closing the gender gap in this field, but also in STEM (science, technology, engineering, and mathematics) in general. In this context, we were responsible for the quality management of the results and outcomes of the reported activities. Being part of the CONCORDIA ecosystem, the Laboratory was also able to connect with other relevant networks and stakeholder groups, such as the ECHO project.

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 raising of the level of digital skills of the European population for all age groups. In this area, the members of the laboratory conducted research and developed solutions for the effective use of educational serious games, which are an integral part of teaching and learning in the field of cybersecurity. A study of the suitability of games and their appropriate classification in terms of technical requirements and the educational level was carried out.

The aim of the 3-year H2020 project "From Research to Policy through Raising Awareness of the State of the Art on Social Media and Convergence (**COMPACT**)" (2017-2020) was to raise awareness (including scientific, political, cultural, legal, economic and technical domains) of the latest technological discoveries among key stakeholders in the context of social media and convergence. The project performed extensive research on policies and regulatory frameworks, as well as pre-standardization efforts in social media for preventing fake news, hate speech, and information disorder, in general. The Laboratory for Open Systems and Networks led the work package for policies and regulatory frameworks, where a methodology for examining the regulatory landscape across the EU countries had been analysed. Concrete policy recommendations were developed for all relevant stakeholders. In 2020, mainly dissemination and exploitation activities were performed as part of the project. In this respect, the results were presented by the laboratory members at several events:

- EuroDIG 2020, where we participated in a Virtual Reality presentation on media and technology convergence;
- The Privacy Days conference, where the COMPACT results were presented in view of the privacy in smart places;
- The DSA/DMA COMPACT Symposium, where we participated in a discussion around the new Digital Services Act;
- The Broken Internet Symposium, where the current state of the Internet architecture and regulations were discussed.

Another topic of interest was research into information understanding in brand building by showing the relationships between the multi-dimensionality of brand orientation, brand-building behaviour and brand identity. In addressing this research question, the study relied on structural equation modelling to validate artefacts, norms and values. The study has practical implications for information sharing in brand building, as it enriches the understanding of the relationships between the reported concepts.

In 2020, in collaboration with several other departments at the Jožef Stefan Institute, we have secured the **Athena** ("Implementing gender equality plans to unlock research potential of RPOs and RFOs in Europe") project, which will start in February 2021. The aim of the project is to establish a system in scientific and higher-educational institutions that enables and ensures gender equality in careers, professional advancement and official positions. As part of the project, we will perform tasks related to the collection and processing of data and the preparation of virtual project events, such as seminars, webinars and conferences.

The Laboratory for Open Systems and Networks is also an active member of the IEEE P2933 Working Group on Clinical IoT standardisation. It 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 definition of the standard development methodology, the taxonomy of the system design and the alignment between the different SGs for integration of their work within the architecture viewpoints. 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 e-health, bringing into the standard the experience and lessons learned from the e-SENS and CONCORDIA architectures for the e-health pilots.

Some outstanding publications in the past three years

1. Jerman-Blažič, Borka, Jerman Blažič, Andrej. Overcoming the digital divide with a modern approach to learning digital skills for the elderly adults. Education and information technologies, ISSN 1360-2357, 2020, vol. 25, no. 1, pp. 259-279.
2. Jerman-Blažič, Borka, Klobučar, Tomaž. Removing the barriers in cross-border crime investigation by gathering e-evidence in an interconnected society. Information & communications technology law, ISSN 1360-0834, 2020, vol. 29, no. 1, pp. 66-81.
3. Gabrijelčič, Dušan, Čaleta, Denis, Zahariadis, Theodore, Santori, Francesca, De Santis, Corrado, Gasparini, Teni. Security challenges for the critical infrastructures of the energy sector. In: SOLDATOS, John (Ed.). Cyber-physical threat intelligence for critical infrastructures security: a guide to integrated cyber-physical protection of modern critical infrastructures. Hanover; Delft: Now publishers. 2020, pp. 226-244.
4. Pavleska, Tanja, Školkay, Andrej, Zankova, Bissera, Ribeiro, Nelson, Bechmann, Anja. Performance analysis of fact-checking organisations and initiatives in Europe. In: TERZIS, Georgios (Ed.). Disinformation and digital media as a challenge for democracy, (European integration and democracy series, Vol. 6). Cambridge; Antwerp; Chicago: Intersentia Ltd. 2020, pp. 217-246.

Organization of conferences, congresses and meetings

1. 26th Slovenian Festival of Science with international participants - Science and technology facing challenges of the time, 10–11 November 2020, (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. INEA/CEF - SI-PASS 2.0.; Integrating Slovenian E-Services with the National eIDAS Node
   Asst. Prof. Tomaž Klobučar
   European Commission
3. H2020 - DEFENDER; Defending the European Energy Infrastructures
   Dr. Dušan Gabrijelčič
   European Commission
4. H2020 - COMPACT; From Research to Policy through raising Awareness of the State of the Art on Social Media and Convergence
   Dr. Tanja Pavleska
   European Commission
5. H2020 - CONCORDIA; Cyber Security Competence Research and Innovation for Research and Innovation
   Dr. Tanja Pavleska
   European Commission
6. H2020 - DE4A; Digital Europe for All
   Asst. Prof. Tomaž Klobučar
   European Commission
7. H2020 - BD4OPEM; Big Data for Open Innovation Energy Marketplace
   Dr. Dušan Gabrijelčič
   European Commission
8. H2020 - iFLEX; Intelligent Assistants for Flexibility Management
   Dr. Dušan Gabrijelčič
   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. Technological and business aspects of future ecosystem for e-health
   Dr. Marina Trkman
   Ministry of Education, Science and Sport
2. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
   Asst. Prof. Tomaž Klobučar
   Slovenian Research Agency

NEW CONTRACT

1. „Use Wisely" project support
   Dr. Dušan Gabrijelčič
   Elektro Celje d. d.

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Original Article

1. Samed Bajrić, "Data security and privacy issues in healthcare", *Applied Medical Informatics*, 2020, **42**, 1, 19-27.
2. Borka Jerman-Blažič, Andrej Jerman Blažič, "Overcoming the digital divide with a modern approach to learning digital skills for the elderly adults", *Education and information technologies*, 2020, **25**, 1, 259-279.
3. Cormac Callanan, Borka Jerman-Blažič, "Privacy risks with smartphone technologies when using the mobile Internet", *ERA-Forum: scripta iuris europaei*, 2020, **20**, 3, 471-489.
4. Borka Jerman-Blažič, Tomaž Klobučar, "Removing the barriers in cross-border crime investigation by gathering e-evidence in an interconnected society", *Information & communications technology law*, 2020, **29**, 1, 66-81.
5. Borka Jerman-Blažič, Tomaž Klobučar, "Investigating crime in an interconnected society: will the new and updated EU judicial environment remove the barriers to justice?", *International review of law computers & technology*, 2020, **34**, 1, 87-107.
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Published Conference Contribution

1. Primož Cigoj, Živa Stepančič, Borka Jerman-Blažič, "A large-scale security analysis of Web vulnerability", In: *ICCSA 2020, Computational Science and its Applications, 20th International Conference, Cagliari, Italy, July 1-4, 2020*, Proceedings, Part V., (Lecture notes in computer science **12253**), Springer, 2020, 763-771.
2. Tanja Pavleska, Helder Aranha, Masi Massimiliano, Giovanni Paolo Sellitto, "Drafting a cybersecurity framework profile for smart grids in EU: a goal-based methodology", In: *EDCC 2020, European Dependable Computing Conference Workshops, AI4RAILS, DREAMS, DSOGRI, SERENE 2020, Munich, Germany, September 7, 2020*, Proceedings, (Communications in computer and information science **1279**), Springer, 2020, 143-155.
3. Marina Trkman, Samed Bajrić, Roko Malkoč, "The success factors of a national healthcare ecosystems maturation: preliminary results", In: *MIPRO 2020, 43nd International Convention on Information, Communication and Electronic Technology, September 28-October 2 2020, Opatija, Croatia*, Proceedings, IEEE, 2020, 977-981.
4. Giovanni Paolo Sellitto, Helder Aranha, Masi Massimiliano, Tanja Pavleska, "Security and safety by design in the internet of actors: an architectural approach", In: *S-BPM ONE 2020, Subject-oriented business process management: the digital workplace-nucleus of transformation, 12th International Conference, Bremen, Germany, December 2-3, 2020*, Proceedings, (Communications in computer and information science **1278**), Springer, 2020, 133-142.
5. Marina Trkman, Božidarka Radović, "Integracija informacijskih sistemov za e-zdravstvo:: študija primera", In: *Umetna inteligenca - korak k večji uspešnosti, 27. konferenca Dnevi slovenske informatike, 27. 10. 2020*, zbornik, Slovensko društvo Informatika, 2020, 48-56.
6. Rok Bojanc, "Analysis of the benefits of e-invoicing", In: *2nd international Eastern European Conference of Management and Economics Workshop on Social Research, May 29, 2020, Ljubljana, Slovenia*, Proceedings, Ljubljana School of Business, 2020, 30-38.

Independent Component Part or a Chapter in a Monograph

1. Dušan Gabrijelčič, Denis Čaleta, Theodore Zahariadis, Francesca Santori, Corrado De Santis, Teni Gasparini, "Security challenges for the critical infrastructures of the energy sector", In: *Cyber-physical threat intelligence for critical infrastructures security: a guide to integrated cyber-physical protection of modern critical infrastructures*, Now publishers, 2020, 226-244.
2. Tanja Pavleska, Andrej Školkay, Bissera Zankova, Nelson Ribeiro, Anja Bechmann, "Performance analysis of fact-checking organisations and initiatives in Europe", In: *Disinformation and digital media as a challenge for democracy*, (European integration and democracy series **6**), Intersentia Ltd., 2020, 217-246.

DEPARTMENT OF COMMUNICATION SYSTEMS E-6

The core activities of the Department of Communication Systems comprise the research, development and design of next-generation telecommunication networks, technologies and services; wireless communication, embedded and sensor systems; and new procedures and algorithms for parallel and distributed computing. Within these activities our research work includes the development of methods and software tools for the modelling, simulation, analysis and synthesis of communication systems, pilots and experimental testbeds, computer simulations supporting biomedical procedures and specialised equipment and procedures for advanced bio-signal processing and interpretation.

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 focused mainly on the research associated with the access segment of radio technologies. We studied radio transmission in terrestrial and satellite communications and management of the radio and network resources. The research is part of the programme on Communication networks and services (P2-0016). Additionally, we were continuing the research in power grids started in previous years and upgrading the LOG-a-TEC testbed with new functionalities.

A significant part of the Communication Technology Laboratory's activities was research in the modelling and simulation of the radio channels. Our focus was on deterministic channel modelling. In this respect we continued to study the ray-tracing algorithms in irregular environments, looking at new approaches and algorithms as well the environment simplification to make radio-wave propagation prediction more time efficient and accurate. In particular, we investigated the performance of ray-tracing techniques in highly irregular environments consisting of many small triangular surfaces, typically obtained by laser scanning. We studied the environment simplification methods, and the best performance was achieved by quadric edge-collapse decimation, which preserves the environment geometry while significantly decreasing the number of surfaces. The optimized description of the radio environment was tested on a 3D natural cave model and a ray-tracing radio-propagation prediction approach. The comparison of the simulated and measured radio signal levels revealed that the proposed approach leads to faster simulation and more accurate simulation results. In the second approach we proposed and evaluated a new method that does not consider only the individual properties of the patches but also the relationships among the neighbouring surfaces, for example, inclination and size, and their relative position to the transmitter and receiver locations.

Based on wireless channel state information we have developed a framework for the estimation, classification and prediction of an indoor environment, which is required for the efficient operation of future intelligent wireless networks.

The deterministic ray-tracing techniques only model a subset of the propagation mechanisms and in their present form do not guarantee appropriate radio channel modelling in the near field of the radio antenna. The massive multiple antenna systems, distributed antennas, the ever-increasing number of access points and closely related reduction of the wireless cell's effective geographical area, as well as the increase in the computational power, opened a new research interest in solving fundamental Maxwell's equations for modelling electrical field also for electrically larger problems. In this respect, we looked at the viability of the numerical full-wave techniques for the telecommunication channel modelling. The acceleration of such techniques for their greater acceptability in electrically large problems is an alternative to the accuracy improvements of existing deterministic models, where ray tracing shows a prevailing trend to replace empirical models. We studied several ways of overcoming excessive time requirements of the numerical approaches while providing acceptable channel modelling accuracy for the smallest radio cells and possibly wider, including the numerical algorithm adaptations for large-scale problems, alternative finite-difference approaches, such as meshless methods, and dedicated parallel hardware.

As part of the research activities in the field of wireless network optimization and management, we studied a novel methodology that enables the prediction of the radio channels' properties beyond what is currently available, by taking the advantage of environmental information, the measured partial channel state information (CSI) and the information about the radio nodes applicable in future intelligent radio networks. This research is the topic of the

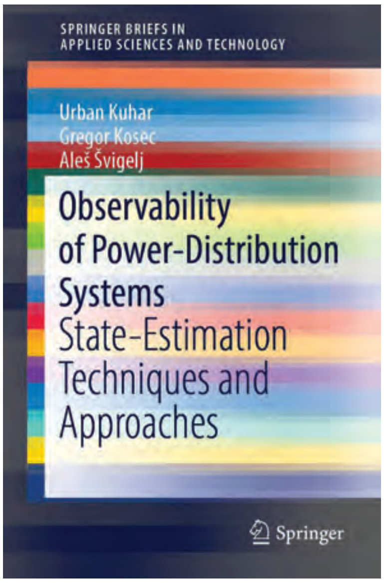

Figure 1: At the Springer publishing house we published a book entitled Observability of Power-Distribution Systems: State-Estimation Techniques and Approaches. The book describes the design and implementation of a three-phase state estimation that is suitable for power-distribution networks.

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 this respect we proposed, studied and evaluated an idea of estimating the 3D environment geometry and electrical properties of the building elements. The idea is based on an assumption that the received radio signal is distorted due to an interaction with the surrounding objects and thus includes the signature of the radio environment. We proposed a novel methodology for how to apply radio environment signatures for the characterization of the geometry and building material of indoor environments by applying machine-learning tools, using ray tracing simulations and ultra-wide band (UWB) communication technology. Computer simulations revealed that wall materials with dissimilar electromagnetic properties can be classified into representative groups observing a single transmission link in the known environment geometry. When the geometry of the environment is not known, more than one radio link has to be included in the learning and testing process. In order to test the hypothesis in a real environment, the handheld tool based on the UWB radio technology was built to estimate the channel state information.

At the outbreak of the COVID-19 epidemic, we became actively involved in 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)). In this approach it is the user who is monitoring the "radio environment" and keeps full control over the collected data, thus preserving anonymity. For this purpose, we developed a mobile application with an associated data platform with which we are collecting the appropriate test data for further modelling.

In 2020 we conducted comprehensive statistical analyses of signal rain attenuation and fade durations obtained from 3 years of measurements of the Alphasat satellite beacons in the Ka-band (19.7 GHz) and the Q band (39.4 GHz) in the ground receiver at the JSI in Ljubljana. Complementary Cumulative Distribution Functions (CCDF) of rain attenuation for each year separately and for 3 years combined were published in a highly ranked journal. The analysis of CCDFs for each separate season shows that higher attenuation values are observed during the summer and spring, compared to autumn and winter, which is due to higher and more intense rain precipitation.

In 2020 we concluded the work in the COST Action 15104 IRACON on "Inclusive radio communication networks for 5G and beyond", where we were contributing to the disciplinary working groups concerned with radio channel, physical layer and network layer, as well as to the experimental working groups on localization and tracking and on the Internet of Things (IoT).

We continued the research in the field of IoT, where we concentrated on the application of the IoT in the industrial environment. In particular we focused on the 6TiSCH standard and its performance evaluation in the LOG-a-TEC wireless testbed, as well as supported external experimentation groups in the investigation of LoRaWAN network performance in RF noise and interference, and the security of IoT networks using 6LowPAN and CoAP protocols.

We summarized our work in the area of smart grids with a book entitled "Observability of Power-Distribution Systems: State-Estimation Techniques and Approaches". The book was published with Springer at the beginning of 2020. It addresses the challenges of future power-distribution systems where the production is shifting from traditional towards renewable sources, while the consumption in the low-voltage grid is expected to grow significantly due to the transition to electrical vehicles. The main focus of the book is the design and implementation of a three-phase state estimation that is suitable for power-distribution networks. It concentrates on the modelling of all the major power-distribution components to enable a three-phase network model's construction. The book is among the most used publications on SpringerLink that look at one or more of the United Nations Sustainable Development Goals in the Affordable and Clean Energy domain. Furthermore, the expertise in signal processing was used in addressing the problem of network topology identification in low-voltage power-distribution grids. We studied the shortcomings of the existing methods and presented some original solutions. Among others, we introduced a topology-identification approach that avoids the assumption of a linearized power flow in order to reduce the sensitivity of the reconstruction process to the measurement errors.

In the **Parallel and Distributed Systems Laboratory** we continued our research of computationally intensive problems and problems for which the computation is distributed over heterogeneous computer architectures. To this end, we have been developing algorithms needed in various fields, from numerical simulations, multi-criteria optimisations and analyses of large amounts of data to graph theory. Our group closely cooperates with the Laboratory of Algorithmics at the Faculty of Computer and Information Science of the University of Ljubljana and the Laboratory for Machine Intelligence at the Faculty of Electrical Engineering of the University of Ljubljana.

We continued developing local meshless methods for the numerical solving of systems of partial differential equations (PDEs), where we are striving to develop a coordinate-free, completely local and sufficiently general approach that can be written in a modular and scalable parallel code. Great attention has been paid to the fusion of the generality of the developed algorithms with generic programming, which is reflected in the Medusa modular open-source library for solving PDE systems. In 2020 we extended Medusa by developing an original parallel algorithm for the discretisation of parametric surfaces, with a solution procedure for the simulation of natural convection of non-Newtonian fluid and with hyperviscosity stabilisation of convection-dominated problems. We also devised a prototype 3D printing simulation for SinusPro GmbH on top of Medusa and initiated research of *hp*-adaptivity.

For the Slovenian power transmission system operator ELES d.o.o., we developed and implemented an algorithm for estimating the uncertainty of the ampacity resulting from the DTR process based on the measurements provided by the client. From the forecast and measurements of weather parameters, we determined their uncertainty and further used Monte Carlo simulations to map it, via the DTR model, into the ampacity uncertainty. In the random simulations we also considered the type and emissivity of the conductor and the forecast horizon, ranging from nowcast to short-term and medium-term forecasts. Since the real-time calculation of the probability distribution of the ampacity is computationally too demanding, we pre-computed the distribution for a set of input data and used a rectilinear homotopy between the closest known distributions to describe the entire state space. Based on the statistical analysis, the algorithm also estimates the conductor load in the N-1 state. The algorithm developed was implemented as an operating module, which we integrated into the client's SUMO system. The module has been in operation since August 2020.

We developed and implemented an algorithm for estimating the uncertainty of the ampacity resulting from the DTR process based on the measurements provided by the client. The algorithm has been in operation in ELES, d.o.o. since August 2020.

By publishing an article, we completed the development of a new algorithm for finding similarities in graph theory. Work in this area will continue in the framework of a bilateral project with Hungary "Graph Theory and Combinatorial Scientific Computing". The main goal of this project is to identify the graph-theoretic problems present in combinatorial scientific computing. Members of the laboratory are collaborating with experts from the fields of theoretical mathematics and computer science from the Institute Alfred Rényi in Budapest, the Universities of Pécz and Szeged, the Faculty of Computer and Information Science of the University of Ljubljana, and the InnoRenew CoE institute.

We started research within the ARRS project "Past climate change and glaciation at the Alps-Dinarides junction", which recognises the markers of past glaciations as important archives for the study of climate change in quaternary. The south-east parts of the Alps and the neighbouring northern Dinarides are not well studied, although the glacial history of this area has been studied since the late nineteenth century. Our work is mostly in dealing with the problem of large disagreements between the empirical reconstructions and numerically modelled simulations of this area. The goals are new findings on how glaciers shaped the landscape and how they reacted to the past climate variability.

We started research within the ARRS project "Decay of an invasive ctenophore bloom as a perturbation to the costal marine microbial community – from molecules to ecosystem – an integrated interdisciplinary approach", in which the leading institution is the National Institute of Biology. Our laboratory deals with the numerical and oceanographic modelling of microbially mediated jellyfish detritus degradation.

In the scope of the SAAM (Supporting Active Ageing through Multimodal coaching) project, we integrated a cardio-vascular module into the SAAM platform. This included connecting the Savvy ECG and a blood-pressure monitor into the SAAM infrastructure and providing services like real-time ECG feature extraction. Additionally, we evaluated the option to use the Savvy ECG in another scenario, i.e., as a part of a system for Personal CARDiac (PCARD) monitoring. All these activities have been conducted to support a cardio-vascular pilot study in SAAM. A preliminary cardio-vascular coaching pipeline was defined, with two scenarios envisioned: irregular rhythm and irregular blood pressure.

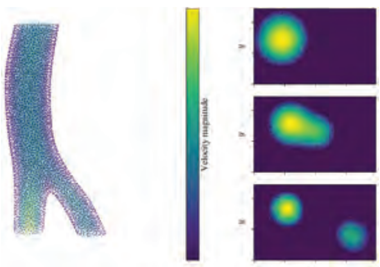

Figure 2: RBF-FD simulation of Non-Newtonian flow through the aorta computed with the Medusa library.

In the field of formal methods for distributed systems, we continued our research of sufficient conditions for the realizability and causal-consistent reversibility of global choreographies.

In the **Networked Embedded Systems Laboratory** we intensified research in the intelligent operation of wireless communication networks as well as continued the research, design, development and implementation of advanced solutions for connecting various things and devices, with the aim to improve their accessibility, utility and efficiency. To this end, we are making use of contemporary concepts such as service-oriented architecture, dynamic service composition, cognitive communications, Internet of Things, machine learning and deep learning. The emphasis is on the vertical integration of different wireless sensor and communication network technologies in support of new applications, making use of the modular platform VESNA as the core building block in the development process and the LOG-a-TEC wireless testbed for testing, experimentation and validation.

The LOG-a-TEC wireless testbed is part of the Next Generation Internet Experimentation (NGI-EXP) initiative (previously FIRE/FIRE+ initiative) through the H2020 Fed4FIRE+ (Federation for FIRE plus) project and also available through a common Fed4FIRE portal to the community of external experimenters. For instance, in 2020 we supported external experimenters in the investigation of zero-touch provisioning and link quality assessment in brownfield industrial deployment. In 2020 the LOG-a-TEC testbed was also upgraded with improved online monitoring capabilities during the experimentation on devices with restricted capabilities in complex wireless operating environments. The implementation is based on modern technologies and frameworks for building distributed web applications interacting with constrained IoT experimentation devices in real time.

In collaboration with Steklarna Hrastnik we developed a smart bottle tag based on NFC and BLE technologies designed to fit in the bottle punt. The smart tag enables improved life-cycle management of glassware and interaction with consumers via advanced visual and infotainment applications.

In 2020 we continued with the research in the H2020 projects DEFENDER, SAAM and RESILOC, the basic research project funded by the Slovenian Research Agency J2-9232 "Resource management for low latency reliable communications in smart grids - LoLaG" and the applied project eBOTTLE with Steklarna Hrastnik. We also started a new H2020 project BD4OPEM.

The DEFENDER project was successfully concluded in 2020. We finished with the design, implementation and verification of advanced data-processing algorithms for the detection, identification and localization of cyber-physical threats based on data from PMU devices deployed in the energy grid. The verified PMU devices were successfully deployed in a real operating pilot environment at the Italian Distribution System Operator ASM Terni for testing and validation. Important measurements on faults in the energy distribution grid were collected within this pilot which will also be used in further research work.

In SAAM we finalized and deployed the algorithms for multimodal activity and context monitoring via the energy consumption of home appliances and interference in the UWB radio channel. We continued upgrading the functionality of individual components and supported further pilot deployments of unobtrusive sensing for monitoring and identifying the activity of the elderly population in real home environments in Bulgaria, Austria and Slovenia.

In RESILOC 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. In particular, we started with the design of (i) a low-cost electronic tag with Bluetooth beaconing for the identification of people and assets; (ii) a mobile app for crowdsensing of people's behaviour in response to new resilience measures; (iii) a Bluetooth and Wi-Fi radio sniffing gateway for 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.

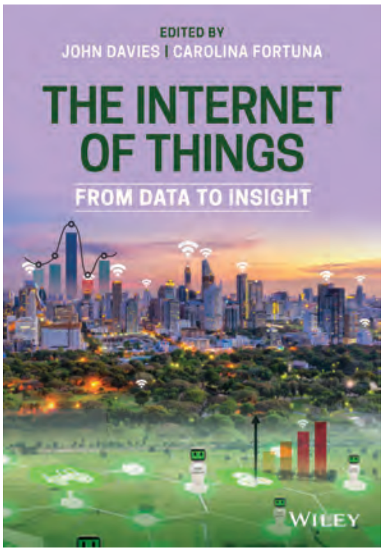

Figure 3: Wiley published a book co-edited by Carolina Fortuna from JSI and John Davies from British Telecom entitled Internet of Things: From Data to Insight. Written by experts in the field, this book addresses the IoT technology stack, from connectivity through data platforms to end-user case studies, and considers the trade-offs between business needs and data security and privacy throughout.

In 2020 we started a new H2020 project "Big Data for OPen innovation Energy Marketplace" - BD4OPEM, which is concerned with developing an analytic toolbox and a set of energy services leveraging currently available yet unutilised big data from the metering, operation and control of energy grids. Our initial work was mainly focused on a detailed investigation and specification of communication solutions with associated standards and protocols that will allow for the instantiation of data and services marketplace and on the definition of use cases. We also contributed to the investigation of data-acquisition channels and technologies and started with the design of solutions for the flexibility aggregation for demand-response, and an energy-management system for smart houses, buildings and industries.

In 2020 we successfully concluded the industrial applied project eBOTTLE with Steklarna Hrastnik, which was concerned with the life-cycle management of glassware. Within the project, we developed functional prototypes of (i) the eBottle smart tag, (ii) a corresponding gateway with reading and wireless charging functionalities, (iii) a backend system for management of data, tags and users, and (iv) web and mobile applications designed for collecting and sending data from tags to the remote database, interrogation with smart tags, and passing the control commands from the remote inventory management system to smart tags.

The above predominantly applied research activities were complemented with basic research in the frame of research programme P2-0016 and ARRS project J2-9232 – LoLaG. In LoLaG we continued with the investigation of ultra-reliable, massive, low-latency communications and edge computing to support real-time monitoring, autonomous protection and the distributed control of smart grids, while in the research programme we continued with the research on data-driven methods for advanced radio resource management, focusing especially on IoT networks. In 2020 we extended the work on automated detection of wireless transmissions to the detection of wireless link anomalies in IoT networks and developed new supervised and unsupervised anomaly detection classifiers with deep learning autoencoder for input features; we continued the work on data-driven link quality estimation (LQE) and developed new supervised LQE classifier; we started with the investigation of life cycle automation of smart infrastructures with the support of artificial intelligence, focusing on deployment automation with the support of zero-touch provisioning; and we were developing advanced edge-cloud computing framework for automated fault localization in energy distribution networks based on phasor measurement unit.

Some outstanding publications in the past year

1. Bedford, Michael Richard, Hrovat, Andrej, Kennedy, Gareth, Javornik, Tomaž, Foster, Patrick R. Modeling microwave propagationin natural caves using LiDAR and ray tracing. IEEE transactions on antennas and propagation, ISSN 0018-926X. [Print ed.], [in press] 2020, 12 pp., doi: 10.1109/TAP.2019.2957969
2. Kuhar, Urban, Kosec, Gregor, Švigelj, Aleš. Observability of power-distribution systems : state-estimation techniques and approaches, (SpringerBriefs in applied science and technology). Cham: Springer, cop. 2020. XV, 108 pp., ilustr., tabele, graf. prikazi. ISBN 978-3-030-39475-2.
3. Rashkovska, Aleksandra, Depolli, Matjaž, Tomašić, Ivan, Avbelj, Viktor, Trobec, Roman. Medical-grade ECG sensor for long-term monitoring. *Sensors*, 2020, vol. 20, no. 6, Article No. 1695, doi: 10.3390/s20061695.
4. Davies, John & Fortuna, Carolina. The Internet of Things: from data to insight, Wiley, UK, 2020, ISBN: 1119545269
5. G. Cerar, H. Yetgin, B. Bertalanič and C. Fortuna, Learning to Detect Anomalous Wireless Links in IoT Networks, in IEEE Access, vol. 8, pp. 212130-212155, 2020, doi: 10.1109/ACCESS.2020.3039333.

INTERNATIONAL PROJECTS

1. CROSSING - Crossing Borders and Scales - An Interdisciplinary Approach
   Dr. Matjaž Depolli
   Helmholtz-zentrum Dresden-rossendorf E.v.
2. COST CA15104; Inclusive Radio Communication Networks for 5G and Beyond (IRACON)
   Prof. Tomaž Javornik
   Cost Office
3. ESA - SatProSi-Alpha; Ka/Q-band Propagation Measurements and Modelling - Slovenian Contribution to the Alphasat TDP#5 Scientific Mission
   Prof. Aleš Švigelj
   Esa/estec.
4. COST CA18203; ODIN - Optimising Design for Inspection
   Prof. Roman Trobec
   Cost Association Aisbl
5. H2020 - Fed4FIREplus; Federation for FIRE Plus
   Prof. Mihael Mohorčič
   European Commission
6. H2020 - DEFENDER; Defending the European Energy Infrastructures
   Prof. Mihael Mohorčič
   European Commission
7. H2020 - SAAM; Supporting Active Ageing through Multimodal Coaching
   Prof. Mihael Mohorčič
   European Commission
8. H2020 - RESILOC; Resilient Europe and Societies by Innovating Local Communities
   Prof. Mihael Mohorčič
   European Commission
9. H2020 - BD4OPEM; Big Data for Open Innovation Energy Marketplace
   Prof. Mihael Mohorčič
   European Commission
10. Joint Scheduling and Routing Algorithm for Delay Sensitive Industrial Applications in Wireless Networks
    Asst. Prof. Andrej Hrovat
    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. Resource management for low latency reliable communications in smart grids – LoLaG
   Prof. Mihael Mohorčič
3. Towards the environment-aware intelligent wireless communications
   Prof. Aleš Švigelj
4. 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
5. Central European SME Gateway zo Key-enabling Technology Infrastructures - Sparking new Transnational KET Innovation Ecosystem
   Dr. Gregor Kosec
   Bay Zoltan Alkalmazott Kutatasi Kozhasznu
6. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
   Prof. Mihael Mohorčič
   Slovenian Research Agency
7. Fusion of ECG and Motion Sensor Data
   Prof. Roman Trobec
   Ruder Bošković Institute

NEW CONTRACT

1. Development and Implementation of Electrical Grid Topology Identification Algorithms
   Asst. Prof. Roman Novak
   Grid Instruments d. o. o.

VISITOR FROM ABROAD

1. Prof. Gordana Gardašević. Faculty of Electrical Engineering, University of Banja Luka, Banja Luka, Bosnia & Herzegovina, February 6.–7. 2. 2020

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1. Antonio E. Saldaña-González, Andreas Sumper, Mònica Aragues-Penalba, Miha Smolnikar, "Advanced distribution measurement technologies and data applications for smart grids: a review", *Energies*, 2020, **13**, 14, 3730.

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Independent Component Part or a Chapter in a Monograph

1. J. Davies, Carolina Fortuna, "Introduction", In: *The internet of things: from data to insight*, Wiley, 2020, 1-7.
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4. J. Davies, Carolina Fortuna, "Conclusion", In: *The internet of things: from data to insight*, Wiley, 2020, 207-212.

Scientific Monograph

1. Urban Kuhar, Gregor Kosec, Aleš Švigelj, *Observability of power-distribution systems: state-estimation techniques and approaches*, Springer, 2020.

Theses and Mentoring

1. Jure Slak, *Adaptive RBF-FD method:* doctoral dissertation, Ljubljana, 2020 (mentor Gregor Kosec).
2. Matevž Vučnik, *Streamlining the development of wireless embedded systems using continuous integration:* doctoral dissertation, Ljubljana, 2020 (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, bioinformatics, 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 keep at the forefront of rapidly developing fields.

Head:
Prof. Gregor Papa

In 2020 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 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 2020 was complemented by the design, development and implementation of various solutions within 11 European projects in *Horizon 2020, ECSEL JU, AAL, COST* and *Interreg* programs, as well as in 12 national projects. Our work is also actively connected to 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 optimisation of several, often time-consuming and conflicting objectives. They might require the use of computational intelligence to maximise the quality while minimising the cost, relying on demanding numerical simulations.

It was the final year of the Horizon 2020 Marie Skłodowska-Curie Actions project *UTOPIAE – Uncertainty Treatment and OPtimisation In Aerospace Engineering* (http://utopiae.eu). The main aim was in bridging optimisation and uncertainty quantification in aerospace systems' applications. Developing fundamental mathematical methods and algorithms to bridge the gap between **uncertainty quantification and optimisation** and between probability theory and imprecise probability theory for uncertainty quantification will lead to efficient solutions of high-dimensional, expensive and complex engineering problems. The second Local Training Workshop of the project was held in person in Milan during February. The Early Stage Researchers (ESRs) – among other activities – held lectures on topics of their research. Our ESR gave a presentation on evolutionary approaches to bilevel optimisation, and a paper on solving min-max optimisation problems by bilevel evolutionary algorithms was presented at the *Genetic and Evolutionary Computation Conference – GECCO 2020* conference. We also hosted an ESR from TH Köln for his secondment in Ljubljana. The final conference of the project was a joint event of the *International Conference on Uncertainty Quantification & Optimisation – UQOP* and ***International Conference on Bioinspired Optimisation Methods and Their Applications – BIOMA 2020*** conferences in November, for which our department was one of the main organisers. The event – besides the challenges of shifting to a fully online event – was held to be a success with numerous participants and interesting presentations. Two papers, related to the work within the UTOPIAE were presented at the *BIOMA 2020* conference.

We organized the 9th International Conference on Bioinspired Optimization Methods and their Applications

To contribute to the more systematic use of **dynamic control parameter** choices for evolutionary computations, we gave three tutorials during the *GECCO 2020*, *IEEE Congress on Evolutionary Computation – CEC 2020* and *Parallel Problem Solving from* Nature – *PPSN 2020* conferences. We surveyed 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.

The main objective of the ARRS research project *Biomedical data fusion by nonnegative matrix tri-factorisation*, in collaboration with the University of Ljubljana and the Institute of Mathematics, Physics and Mechanics, was the development of new, efficient and accurate methods for **non-negative matrix tri-factorisation** problems applied to real-world, complex biomedical data. The aim of its application is to search for previously unknown associations in biomedical data. Such associations can lead to further patient stratification, the discovery of new disease biomarkers, drug repurposing and similar. The project has finished with a paper that summarises the main project results. The developed methodology is an important data-mining technique applicable in data clustering, representation learning, data fusion, similarity learning and data compression.

In an ARRS young researcher project the focus was on applying **gradient-based methods** to machine learning and large-scale optimisation. The exploration of the effectiveness of gradient-based methods was performed in all three 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 *PRACE Autumn school 2020 – HPC and FAIR Big Data* in Ljubljana, Slovenia.

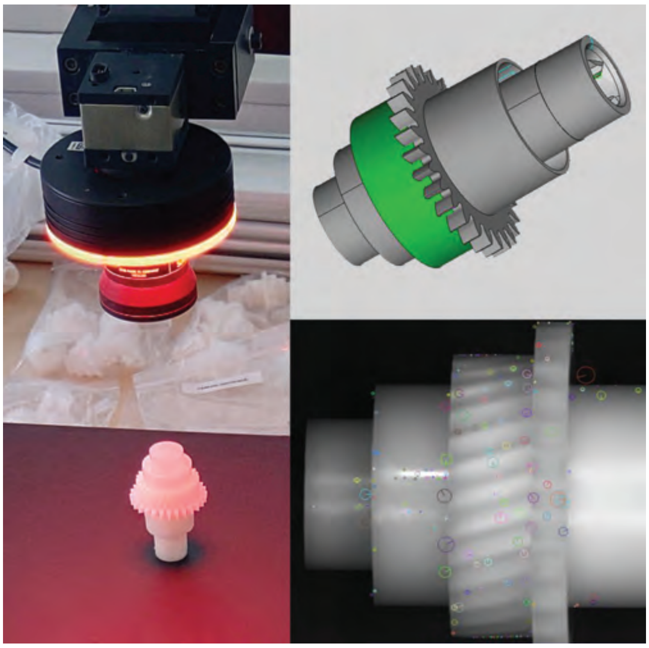

Figure 1: Machine vision for product quality control

Another ARRS young researcher project was focused on algorithms, benchmarking, **exploratory landscape analysis**, data visualization and machine learning. The related paper was accepted and published in the *Applied Soft Computing* journal, and was additionally presented at the *GECCO 2020* conference.

Within ARRS post-doc funding for the project *Mr-BEC – Modern approaches for Benchmarking in Evolutionary Computation* (http://cs.ijs.si/project/mrbec) the main objective is to invent, develop, implement, and evaluate a **framework for benchmarking in evolutionary computation**, which will consist of methodologies that will bring about an in-depth understanding of an algorithm's behaviour, especially focusing on identifying practical significance, obtaining knowledge about performance using the information from space distribution (high-dimensional data), and making a more general benchmarking conclusion using a set of performance metrics. All the developed approaches within the project have been integrated in the *IOHAnalyzer*, a benchmarking framework developed by Leiden University, the Netherlands, and the Sorbonne University, France. The work related to identifying practical significance in benchmarking was presented at the *GECCO 2020* conference. Also, a special session and two workshops on benchmarking practices for evolutionary computation were organized at the *GECCO 2020* and *Parallel Problem Solving from Nature – PPSN 2020* conferences. Two additional tutorials related to the benchmarking approaches have been organized at these two conferences. This research on benchmarking also contributed to several below-mentioned journal papers.

When making a statistical analysis of single-objective optimization algorithms' performance, researchers usually estimate it according to the obtained optimization results in the form of minimum/maximum values. Though this is a good indicator about the performance of the algorithm, it does not provide any information about the reasons why it happens. One possibility to get additional information about the performance of the algorithms is to study their exploration and exploitation abilities. We have shown, by the use of **extended Deep Statistical Comparison** approach, which works with high-dimensional, how exploration and exploitation analysis of single-objective optimization algorithms can be performed. The pipeline is based on a web-service-based e-Learning tool *DSCTool*. The work was published in the *Mathematics* journal.

Multi-objective optimization is one research area where proper usage of statistics is important, since the performance of a newly developed algorithm should be compared with the performances of state-of-the-art algorithms. In multi-objective optimization, we are dealing with two or more usually conflicting objectives, which result in high-dimensional data that needs to be analysed. In the *Mathematics* journal we reported how to perform a proper statistical analysis for multi-objective optimization.

Our department took part in the *Open Optimization Competition* organized at the *GECCO 2020* and *PPSN 2020* in the direction of more robust statistical measures and visualization of the optimization results. Our team was **ranked first at the competition**. The work also resulted in two papers presented at the *GECCO 2020*.

The work in collaboration with Sorbonne University, Institut Polytechnique de Paris focused on using matrix factorization to represent benchmark problem instances that are used in performing benchmarking studies in order to find more similar instances. This was presented at the *IEEE International Series Symposium on Computational Intelligence – IEEE SSCI*. The developed benchmarking approaches have also been used to provide in-depth insights of swarm intelligence algorithms performance in collaboration with the Singidunum University, Serbia, which was presented at *Modelling and Development of Intelligent Systems 2020 – MDIS 2020* conference.

The work on the *performance2vec* representations was presented at the *GECCO 2020*. Performance2vec is used to represent a performance embedding of an algorithm on a given benchmark data set. In this way we can identify which algorithms perform similarly and which algorithms from a selected algorithm portfolio are suitable for particular optimization problems.

We finished with the activities within COST Action *ImAppNIO – Improving Applicability of Nature-Inspired Optimisation by Joining Theory and Practice* (http://imappnio.dcs.aber.ac.uk). The main objective of the Action was to bridge this gap and improve the applicability of all kinds of nature-inspired optimisation methods. It made theoretical insights more accessible and practical by creating a platform where theoreticians and practitioners can meet and exchange insights, ideas and needs. Our researchers actively participated at the final MC meeting and working group workshop, held in Vilnius, Lithuania. The working group on Practice-Driven Theory focused on the combinatorial optimisation and medical applications. Related to the suggested topic some results obtained at the project *Biomedical data fusion by nonnegative matrix tri-factorization* were presented.

Our team was ranked first at the Open Optimization Competition organized at the GECCO 2020 and PPSN 2020 conferences

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 seventeenth consecutive year, the *Nature-inspired algorithms* workshop dealing with stochastic optimisation techniques.

We collaborate with the Department of the Environmental Sciences at JSI within several projects by performing classic statistical analyses and machine-learning models that can be used to identify food traceability.

Data processing

In 2020 we have successfully concluded the Ket4CleanProduction industrial project *Improved planning of manufacturing processes for individualized tools*. The main objective was to improve the estimation of operation durations of highly individualized actions at Plamtex d.o.o. tool production process using an **Artificial Intelligence based analysis**. We addressed two main challenges. The first one was the creation of features that can be used for AI-based modelling, where the main issue was the data format in which all the information about the tools were stored. The second challenge was a correct estimation of the duration of the production process steps for a tool design where an individual tool has never before been produced. The work was being carried out in collaboration with Department of Intelligent Systems at the JSI and the company Hahn-Schickard, Germany. The solution was implemented at the Plamtex tool-shop as system prototype demonstration in an operational environment. It provides a holistic solution to support the planning of tool manufacturing operations by means of AI in the form of automatically constructed (i.e., built through data mining) predictive models.

Electronic components and systems (ECS) are essential to the economy and citizens of the EU, supporting 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 have 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 ECS all along the value chain. Within the project we will focus on securing reliability through the application use case titled Smart condition monitoring for the in-wheel propulsion system. We will develop, customize and implement AI-based algorithms with the goal of identifying the critical parameters that impact the reliability of in-wheel electric motors.

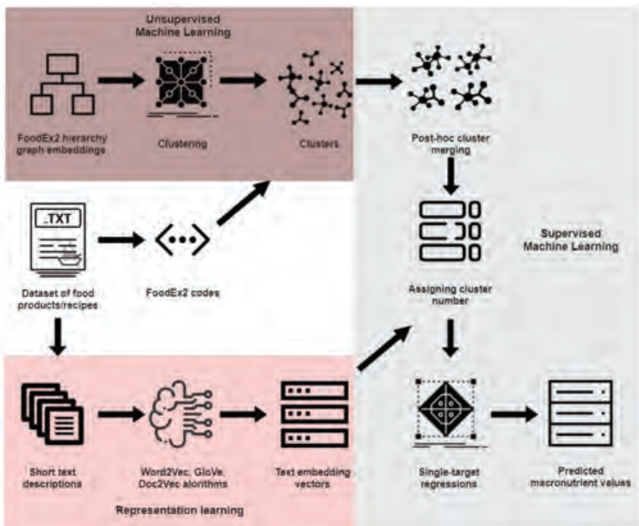

Figure 2: P-NUT methodology

Benchmarking approaches have been used to analyse the COVID-19 pandemic on the food consumption process working with semantic annotation AI approaches for handling recipes' textual data. The work in collaboration with Knowledge Technologies Department was published in the *Trends in Food Science & Technology* journal. These approaches have also been used to develop a framework for selecting the pre-processing parameters of ECG signals used for blood pressure prediction, in collaboration with the Ss. Cyril and Methodius University, Skopje, North Macedonia. The work was published as a chapter in the *Springer Communications in Computer and Information Science book series*.

In collaboration with the Faculty of Computer Science and Engineering, Ss. Cyril and Methodius - University, Skopje, North Macedonia we developed the first open-source end-to-end system for **text-to-speech synthesis** in the Macedonian language. The developed model is known as *MAKEDONKA* and is based on a deep-learning model. The work is published in *Applied Sciences* journal.

Another ARRS young researcher project started in October 2020. Its main goal is to develop an approach that will provide the most suitable **representation learning** (RL) method (especially graph-based RL) for a new data set and a given machine learning (ML) task. One of the subgoals is to develop a new RL fusion approach trying to combine different subspaces where the same data is represented in order to achieve better explainable performance. This will allow developing explainable taxonomy of RL methods that can help researchers select the relevant method for their ML task. To evaluate the developed methods, an evaluation will be performed working with data from food and nutrition and biomedical domain. Additionally, to make a generalization, social and other domains will be also used for testing purposes.

We are building high-performance hybrid GPGPU / FPGA acceleration infrastructure

Within our research on machine-vision quality control we successfully carried out the industrial Ket4CleanProduction project *Machine vision quality control of molded plastic parts*. The goal of the project was to specify and to verify with production data all the elements needed to manipulate and to inspect the specific product, the plastic worm wheel, that is being produced by injection moulding. Our role was to coordinate the research partners and to specify all the necessary components of the machine vision inspection system. The project was implemented in four tasks. In the first task a solution was found for retrieving moulded parts from the moulding machine and for handling them in front of the machine-vision camera in order to enable the collection of the images needed for the quality control. In the second task all the necessary components of the machine-vision inspection system, including their interaction and communication with the product manipulation system, were specified. In the third task **image processing, feature selection and classification** algorithms for quality control of the selected moulded part were defined, selected and tested. In the fourth task the control signals for all phases of the visual inspection were specified and a suitable timing diagram was generated. The main impact achieved with this project is the model solution for the visual inspection and manipulation of plastic products with the robots.

As part of the data pre-processing and data curation and annotation, work on **automated food image recognition** has been done. At the *DSM Science and Technology Award Symposium* that was organised as part of the *European Nutrition Conference*, which focuses on personalised nutrition and novel technologies for health in the modern world, our work was recognised as one of three best works. We also attended the *Food Recognition Challenge* organised by AICrowd, where we achieved second place. The goal of this challenge was to train models that can look at images of food items and detect the individual food items present in them.

For an industrial partner we developed a proof-of-concept pipeline for image-based recognition of their products on a mobile device, including OCR. The solution is intended for end-customers who use the products during their home leisure activities, where robustness and ease of use are essential.

Data management and visualization

We continued with the upgrade of the national food-composition database and further development of the *Open platform for clinical nutrition – OPEN* (http://www.opkp.si). The upgrades include a review of existing data, inclusion of new FNS databases, new and improved classification and mapping of data in FoodEx2. Until now, we have redesigned its underlying food composition database and developed a new user interface for maintaining the database. Related to OPEN, we worked on the **crowd-sourcing platform** for gathering food composition data for packaged products available on the Slovenian market. The platform is composed of the iOS and Android applications *Veš, kaj ješ?* and the web application for editing users-sent data *www.bazil.si*. Firstly, efforts were focused on increasing the stability and usability of the system and secondly, work started on the inclusion of additional data to allow giving the public information about the risks related to alcohol consumption and thw inclusion of sweeteners and caffeine. This work is funded by two national projects: *Veš kaj ješ?* and *Veš kaj piješ?* (http://www.veskajjes.si).

We also continued with the Horizon 2020 project *FNS-Cloud – Food Nutrition Security Cloud* (http://www.fns-cloud.eu). During the project, we will consolidate the existing FNS resources (data, knowledge and tools) for health and agri-food sciences, which are fragmented, lack critical mass, and their access by user communities is 'unevenly' distributed. In particular, we will develop an advanced methodology for work with heterogeneous data on food, nutrition and health. Our group is working on methodologies for data standardisation and the **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 project, two workshops, *Big Food and Nutrition Data Management and Analysis – BFNDMA 2020* at the *IEEE BigData 2020* and *AI & Nutrition Track* at the *Applied Machine Learning Days – AMLD 2020*, were organized. In addition, we are also working with project partners in the field labs and demonstrators within the project where the usefulness of FNS-Cloud will be demonstrated within a family-meal planning and seed-exchange scenarios.

By using a short recipe description, a **new data-mining pipeline** has been developed, *P-NUT*, for predicting macronutrient results, and was published in the *Mathematics* journal. Besides, a bias analysis to investigate the impact of different domain knowledge on the P-NUT predictions has been conducted, and the results have been published and presented at the *BFNDMA 2020* workshop at the *IEEE BigData 2020*.

An evaluation of four different named-entity recognition (NER) methods in the food domain: FoodIE, NCBO (SNOMED CT), NCBO (OntoFood), and NCBO (FoodON) has been made on a data set of 1000 manually annotated recipes. It is evident that FoodIE, our 2019 proposed method, provides more promising results for each particular evaluation metric, as well as the best overall result. These results have been published in the *IEEE Access* journal. Furthermore, to allow **automatic annotations**, we introduced *BuTTER*, which is the first corpus-based food NER method that is based on a bidirectional long short-term memory network with a conditional random field layer and provides more robust results. The approach has been published and was presented at the *BFNDMA 2020* workshop at *IEEE BigData 2020*.

A new **semantic annotation methodology**, *DietHUB*, for recipes' analysis has been developed and published in the *Trends in Food Science & Technologies* journal, in collaboration with the Department of Knowledge Technologies at JSI. This approach allows us to investigate the COVID-19 pandemic's impact on food-consumption patterns, which has also been published in the same journal and presented at the *European Open Science Forum – ESOF 2020* in Trieste, Italy.

To make links between different food standards understandable by food-subject-matter experts and to make them familiar with the interoperability process using different standards, we developed *FoodViz*, which is a web-based framework aimed for presenting food annotation results from existing **Natural Language Processing** and Machine-Learning pipelines in conjunction with different food semantic data resources. FoodViz allows users to filter recipes by the name, by the recipe category and between the curated and un-curated recipes. Then the user can select a recipe, for which the semantic annotations are shown. For each extracted food entity the synonyms are presented, which are the food names available in different food semantic resources, followed by semantic tags. The tool was developed in collaboration with the Faculty of Computer Science and Engineering, Ss. Cyril and Methodius - University, Skopje, and has been published and presented at the *Machine Learning, Optimization, and Big Data – LOD 2020*.

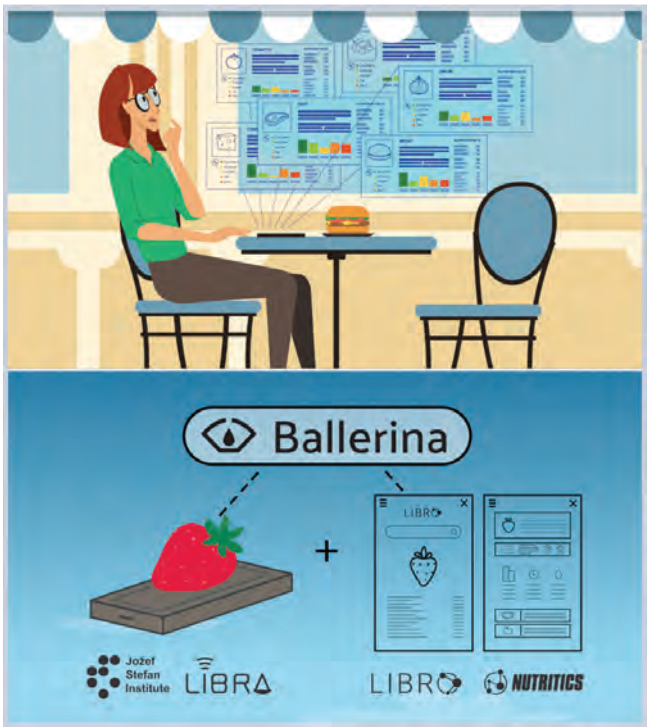

Figure 3: Ballerina presentation video (https://www.youtube.com/watch?v=hi-gT7ljuQc)

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 have developed a **web-based tool for exploring isotopic data**, named *RealMed*. Our department has contributed to the design of the architecture of the MetroFood platform as well as to its data-management plan.

We collaborate with the research group at the Milko Kos Historical Institute of the Research Centre of the Slovenian Academy of Sciences and Arts within the ARRS project *Toponomastical Heritage of Primorska Region*. One of the main results is a reliable **interactive** version of the Slovenian Historical Topography.

In the area of **efficient interaction systems**, we focused on the web tools for nutrition and food informatics. We thoroughly investigated and designed visual representations for various projects, applications, and web pages. In collaboration with partners and end-users, we analysed user needs and defined appropriate user experiences and designed corresponding interfaces for several tools related to nutrition. Within the AAL program *Turntable – Platform supporting vitality and abilities of elderly* (https://www.aalturntable.eu) project we havve collaborated in the co-creation sessions (completed the sessions in Slovenia as one of the four testing countries) where elderly people were asked their opinion on ICT tools to be integrated within the Turntable platform. Within the Interreg program we started the *SI4Care* project, with the aim to create a transnational effective ecosystem for the Social Innovation application in integrated healthcare services for the ageing population across ADRION countries. Our role is piloting some of our ICT solutions developed within other projects and contribute to the decision-support system for evaluation social innovation status in the region.

In October we co-organized the *Human-Computer Interaction in Information Society – HCI-IS* conference in Ljubljana (held virtually). The aim of the conference was to bring together the HCI community in the region.

Given the rising number of participants in this fifth edition of the conference both from most academic institutions working in the field in Slovenia as well as participation from industry, we see that we have succeeded in our aim.

We continued with the upgrade of our *OPEN platform*. Within this, the user interface for managing our internal nutrition database, which is being filled with data from multiple ongoing projects covering different aspects of nutrition research was improved. Our goal is to provide the system administrators and nutrition experts with an easy way to browse through data, obtain the needed insights and edit or connect multiple items based on these insights. Therefore, we designed special user interfaces that enable users to connect food items, categories, components and tags between multiple imported food databases (European, USA, Australian, etc.). We designed the screens in a way that provide users with the means of simultaneously searching and scanning the lists of different databases and then simply click on the appropriate results, connecting them into the chain of data, which is stored and used in our internal database. We furthermore designed an **intuitive way** to review each item stored in our database and make the appropriate edits quickly, thanks to the interface that reduces the needed clicks and allows an easy way to jump review a vast amount of items in a glance.

We designed the *SnackTrack* application user interface to test how certain visual elements on the mobile screen affect the users' choice of food in their daily life. The interface has been designed, but the social experiment, part of the PhD thesis, is currently on-hold due to COVID restrictions. The goal is to build different application instances to test if they affect the nutrition of people when using them differently. We chose photos which we would intend to influence the food choices of people (making them different between instances of the app). From user interface perspective we establish a system that provided users with a quick and easy way to track and tag each meal they ate in a day with as little effort as possible (while still receiving all the relevant data needed for the nutrition analysis). A similar application, *SnackCheck*, requires the users to track their meals as well and uses the gathered data for training image recognition algorithms based on the tags the users provide.

Within the national project *School pot* (http://solskilonec.si) we started designing a new user interface for a meal-planning tool to be used in schools. Our goal is to enable users to **plan the balanced meals** that are consistent with national nutrition guidelines. We designed interactive visualizations that help users determine the appropriate quantities of specific macro- and micro-nutrients and other parameters. We provided multiple ways for achieving this – with automatic import from another system they already use and then guiding them with the interface through confirming imported data; searching and inputting multiple food items from our database and modifying them when possible; and providing a quick way to manually input the needed data from their own food items. We specifically designed screens to manage data about recipes they intend to use and group users that they intend to feed. We presented the calculated quantity in a clear form and visualized how well their designed menus follow national nutrition guidelines. We connected this tool with our *OPEN* database as well as with *e-Katalog*, the tool developed by the Chamber of Agricultural and Food Enterprises, aimed for public procurement of food in schools and kindergartens.

Within the Horizon 2020 project *TRUE – Transition paths to sustainable legume based systems in Europe* and in collaboration with the Knowledge Technologies Department at the JSI we designed the user interface of Pathfinder, a tool for **managing the sustainability** of certain food chains in a holistic way including all relevant aspects: environmental, economic and social. Our goal was to enable the government officials and company managers to obtain a clear view into the condition of all aspects of sustainability and make appropriate changes based on the insights they attain when they are testing different scenarios with our tool. Therefore, we provided interfaces supporting different workflows. One provides an easy way for infield workers to quickly input their indicators of the value chain into our system. We did this by designing the screens to communicate specific ranks of different parameters with maximum clarity and at the same time provide users a clear sense of all the indicators they need to input to successfully finish the task. The other part of the interface is aimed at providing an overview of all indicators with clear, colourful and interactive visualizations. The last part of the interface allows an intuitive way of performing bottom-up and top-down analyses and testing of different scenarios. This means we provided a quick way to subsequently change multiple parameters and see the consequences, and we allowed companies and governments to determine the sustainability goals they want to achieve and then display the possible combinations of parameters this goal can be achieved with.

Adaptive computing platforms

To support and accelerate our algorithms, several approaches were studied and developed on the level of hardware and computing structures, which includes the use and online reconfiguration of FPGAs, customized embedded systems and sensors. We 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 usage of high-performance ALVEO FPGA acceleration card was investigated for the fixed-point array multiplication, which can be used in ANN. The work is documented in the master's thesis by one of our students. Similarly, as part of one Bachelor's thesis, Fast Binary Neural Network architecture was implemented on a medium-size FPGA device. Such a solution is suitable for real-time edge applications. In November we also organized a seminar on the Embedded systems development using FPGA devices.

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 the topic of the numerical simulation of condensation-induced water hammers, which cause serious damage in industrial facilities. Our main task is to investigate the possibilities to implement a class method on **graphical processor units** (GPU) and the application of suitable machine-learning methods to significantly reduce the computing time. In real-world systems we often need to simulate the behaviour of multiple liquids/solids and interactions between them. The simulations can be arbitrarily complex by including different physical phenomena making the simulations more or less accurate. One mechanism of interest is also modelling the size of the bubbles inside a liquid. To simplify the computation, bubbles are usually represented with a discrete distribution. Multiple mechanisms can then change this bubble distribution over time. Two of the most important mechanisms are bubbles merging into a bigger one (coalescence) and bubbles breaking up into smaller bubbles (breakup). The mechanism is extremely computationally expensive. The computation of these two mechanisms was transferred to the GPU. As a result, the GPU-supported physical mechanism can run up to seven times faster. The total computational time of some simulations was reduced by a few hours, which allows faster prototyping with existing models and can speed up new model development.

We continued with the Horizon 2020 project *TETRAMAX – Technology Transfer via Multinational Application Experiments* (https://www.tetramax.eu) and the activities of related to *Ballerina* (http://ballerina.ijs.si), where we have developed a new **energy-efficient pocket-size** kitchen scale with a Bluetooth 5 interface. The API interface of the scale is backwards compatible with previous versions and it was extended to allow Over-The-Air update. The core of the pocket kitchen scale is based on Nordic nRF52 Bluetooth micro-controller with separate precise ADC converter for accurate weight measurement. The scale also includes a power-supply management unit and a UART interface for debugging purposes. The power consumption is reduced by switching off unused modules and by switching the micro-controller to low power sleep mode when idle. The hardware of the scale, the API interface, and testing mobile app are licensed as open source and are provided on request. The Ballerina results were presented at the *HiPEAC 2020* conference.

Within the Horizon 2020 project *SAAM – Supporting Active Ageing through Multimodal coaching* (http://bilsp.org/saam-active-ageing) a methodology for estimating food and nutrient intake of seniors was developed. A short food-frequency questionnaire for seniors was prepared and a mobile (Android) app for taking and recognizing food and drink from photos was tested. To improve the estimation of food and nutrient intake the mobile app connects to the pocket size kitchen scale which was upgraded to support the latest Bluetooth technology. Within the project an **ambient sensor** was also developed. It is a headless system that collects environmental data, like temperature, humidity, pressure, and acceleration from sensor board. Additionally, it collects motion data from wearable sensors via Bluetooth interface. Acquired data are transmitted to the coaching database system using MQTT protocol. Besides data acquisition the ambient sensor integrates 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 MQTT protocol and it plays pre-recorded messages. Voice command module detects audio commands and sends them to the system.

Mobile computing evolution is critically threatened by the limitations of battery technology, which does not keep pace with the increase in energy requirements of mobile applications. In our research we strive to identify the opportunities for adaptable computation that in a controlled manner sacrifices some of the computational accuracy in cases when a user is satisfied with the sub-optimal result. Minimising this gap between the user's expectations and the delivered quality of computation opens new opportunities for saving energy on a mobile device, i.e., the **approximate mobile computing** (AMC) approach. The first step towards realising AMC is to identify the situations in which a user tolerates reduced-accuracy results. In our work on mobile video perception analysis, published at the *EAI MobiQuitous 2020* conference, we have examined how different video playback quality levels are tolerated in different contexts of use. We conducted a user study to investigate how the context in which a video is played modulates a user's quality expectations. We discover that a user's physical activity and the spatial/temporal properties of the video interact and jointly influence the minimal acceptable playback resolution. Further, we confirmed that video decoding resolution can indeed play a significant role in reducing the overall power consumption of a mobile device, thus we propose context-dependent dynamic video quality adaptation as the first step towards realising AMC.

In the frame of the Horizon 2020 *TETRAMAX* project supporting the European *Smart Anything Everywhere* 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. We organized an online workshop aimed at the local community in Slovenia to explain the TETRAMAX mission and present open calls, identify regional "smart specialisation", and to capture the local supply and demand for the

CLEC technologies. In cooperation with SRIP SC&C and SRIP FoF we carried out two technical educational courses, on topics considering Human-Computer Interaction techniques and the built-in systems with FPGAs, to present some key CLEC technologies to SMEs and mid-caps.

Some outstanding publications in the past year

1. Urban Škvorc, Tome Eftimov, Peter Korošec, "Understanding the problem space in single-objective numerical optimization using exploratory landscape analysis", *Applied soft computing*, ISSN 1568-4946. 2020, vol. 90, pp. 106138-1-106138-15, doi: 10.1016/j.asoc.2020.106138.
2. Gordana Ispirova, Tome Eftimov, Barbara Koroušić Seljak, "Evaluating missing value imputation methods for food composition databases", *Food and chemical toxicology*, ISSN 0278-6915, 2020, vol. 141, pp. 111368, doi: 10.1016/j.fct.2020.111368.
3. Gorjan Popovski, Barbara Koroušić Seljak, Tome, Eftimov, "A survey of named-entity recognition methods for food information extraction", *IEEE access*, ISSN 2169-3536, 2020, vol. 8, pp. 31586-31594, doi: 10.1109/ACCESS.2020.2973502.
4. Monika Simjanoska, Stefan Kochev, Jovan Tanevski, Ana Madevska Bogdanova, Gregor Papa, Tome Eftimov, "Multi-level information fusion for learning a blood pressure predictive model using sensor data", *Information fusion*, ISSN 1566-2535, 2020, vol. 58, pp. 24-39, doi: 10.1016/j.inffus.2019.12.008.
5. Veljko Pejović, Artemis Skarlatidou, "Understanding interaction design challenges in mobile extreme citizen science", *International journal of human-computer interaction*, ISSN 1044-7318, 2020, vol. 36, pp. 251-270, doi: 10.1080/10447318.2019.1630934.
6. Veljko Pejović, "Towards a holistic net neutrality violation detection system: a case study of Slovenia", *Journal of network and systems management*, ISSN 1064-7570, 2020, vol. 28, pp. 1453-1481, doi: 10.1007/s10922-020-09546-9.
7. Peter Korošec, Tome Eftimov, "Multi-objective optimization benchmarking using DSCTool", *Mathematics*, ISSN 2227-7390, 2020, vol. 8, pp. 839-1-839-14, doi: 10.3390/math8050839.
8. Gordana Ispirova, Tome Eftimov, Barbara Koroušić-Seljak, "P-NUT: Predicting NUTrient content from short text descriptions", *Mathematics*, ISSN 2227-7390, 2020, vol. 8, pp. 1811-1-1811-21, doi: 10.3390/math8101811.
9. Tome Eftimov, Gorjan Popovski, Matej Petković, Barbara Koroušić-Seljak, Dragi Kocev, "COVID-19 pandemic changes the food consumption patterns", *Trends in food science & technology*, ISSN 0924-2244, 2020, vol. 104, pp. 268-272, doi: 10.1016/j.tifs.2020.08.017.

Awards and Appointments

1. Dr. Tome Eftimov, Rok Hribar, univ. dipl. fiz., prof. dr. Peter Korošec, Gašper Petelin, mag. inž. rač. in inf., Gorjan Popovski, mag. inf. in kom. teh., Urban Škvorc, mag. inž. rač. in inf. took 1st place in the competition organized as part of the GECCO 2020 (GECCO Open Optimization Competition 2020): "Deep statistic: more robust performance statistics for single – objective optimization benchmarking". The award was given by The Nevergrad and the IOHprofiler team (https://github.com/facebookresearch/nevergrad/blob/master/docs/opencompetition2020.md)
2. Simon Mezgec, mag. inž. rač. in inf. won 2nd place in the Food Recognition Challenge competition organized by AIcrowd (https://www.aicrowd.com/challenges/food-recognition-challenge/leaderboards?challenge_round_id=261)

Organization of conferences, congresses and meetings

1. AI & Nutiriton track at Applied Machine Learning Days 2020 (AMLD 2020), Lausanne, Switzerland, 26.–29. 1. 2020
2. FNS-Cloud workshop: "Food and nutrition ontologies", Ljubljana, 20. 2. 2020
3. Online workshp TRAMAX: "Preparation of a successful business model from an open tender for entrepreneurial projects within TETRAMAX", Ljubljana, 9. 6. 2020
4. The Good Benchmarking Practices for Evolutionary Computation (BENCHMARK@GECCO) Workshop, (online), 8.–12. 7. 2020
5. Special Session on Benchmarking of Evolutionary Algorithms for Discrete Optimization (BEADO), IEEE Congress on Evolutionary Computation (IEEE CEC), (online), 20.–24. 7.2020
6. 36th Slovenian workshop "Algorithms by Nature Models", (online), Maribor, 29. 9. 2020
7. Human-Computer Interaction in Information Society (HCI-SI), Ljubljana, 7.10.2020
8. Online workshop TETRAMAX: "User interface design - practical guidelines", Ljubljana, 14. 10. 2020

9. Lorenz Workshop: Representation Learning meets Exploratory Landscape Analysis: BENCHMARKED: Optimisation meets Machine Learning, 9.–11. 11. 2020
10. BIOMA 2020 Conference, The 9th International Conference on Bioinspired Optimisation Methods and Their Applications, BIOMA 2020, Brussels, Belgium, 19.–20. 11. 2020 (online)
11. Online workshop TETRAMAX: “Embedded systems with FPGA circuits”, Ljubljana, 25. 11. 2020
12. Workshop: Big Food and Nutrition Data Management and Analysis (BFNDMA 2020), IEEE International Conference on Big Data 2020 (IEEE BigData), 10.–13. 12. 2020, (online)
13. 37th Slovenian online workshop “Algorithms by Nature Models”, Ljubljana, 2. 12. 2020
14. The Good Benchmarking Practices for Evolutionary Computation (BENCHMARK@PPSN) Workshop, online, 5.–9. 12. 2020
15. FNS-Cloud workshop: “Food and nutrition ontologies – advance module”, Ljubljana, 18. 12. 2020

Patent granted

1. Gregor Papa, Barbara Koroušić-Seljak, Marko Pavlin, Device and method for acquisition and transfer of signals, GB2525403 (B), UK Patent Office, 23. 12. 2020.

INTERNATIONAL PROJECTS

1. CROSSING - Crossing Borders and Scales - An Interdisciplinary Approach
   Prof. Gregor Papa
   Helmholtz-zentrum Dresden-rossendorf E.v.
2. COST CA15140 - ImAppNIO; Improving Applicability of Nature-Inspired Optimisation by Joing Theory and Practise
   Dr. Vida Vukašinović
   Cost Office
3. H2020 - UTOPIAE; Uncertainty Treatment and OPtimization in Aerospace Engineering
   Prof. Gregor Papa
   European Commission
4. 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
5. H2020 - TETRAMAX; TEchnology TRAnsfer via Multinational Application eXperiments
   Dr. Marina Santo Zarnik
   European Commission
6. H2020 - SAAM; Supporting Active Ageing through Multimodal Coaching
   Prof. Barbara Koroušić Seljak
   European Commission
7. H2020 - FNS-Cloud; Food Nutrition Security Cloud
   Prof. Barbara Koroušić Seljak
   European Commission
8. H2020 - METROFOOD-PP; METROFOOD-RI Preparatory Phase Project
   Prof. Barbara Koroušić Seljak
   European Commission
9. H2020 - iRel40; Intelligent Reliability 4.0
   Prof. Gregor Papa
   European Commission
10. H2020 - InSecTT; Intelligent Secure Trustable Things
    Dr. Drago Torkar
    European Commission

RESEARCH PROGRAMME

1. Computer Structures and Systems
   Prof. Gregor Papa

R&D GRANTS AND CONTRACTS

1. Toponomastical heritage of Primorska Region
   Asst. Prof. Jurij Šilc
2. Strategic Research & Innovation Partnership Factories of the Future (SRIP PMIS)
   Prof. Gregor Papa
   Ministry of Economic Development and Technology
3. Support for Strategic Research and Innovation Partnerships (SRIP) in priority areas of Smart Specialization
   Prof. Gregor Papa
   Ministry of Economic Development and Technology
4. 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
5. 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
6. empSupport for Strategic Research and Innovation Partnerships (SRIP) and priority areas of Smart Specialization
   Dr. Bojan Blažica
   Ministry of Health
7. 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
8. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
   Prof. Gregor Papa
   Slovenian Research Agency

NEW CONTRACTS

1. Capsule recognition method development, Android application implementation
   Dr. Bojan Blažica
   BSH Hišni aparati d.o.o.
2. Improved production process planning for individualized tools
   Prof. Peter Korošec
   PLAMTEX INT., trgovina in proizvodnja, d.o.o.
3. Machine vision quality control of molded plastic parts
   dr. Drago Torkar
   MPT, d.o.o.

VISITORS FROM ABROAD

1. Prof. dr. Paul Glen Flikkema, North Arizona University, Department of Electrical Engineering and Computer Science, North Arizona, USA 1. 10. 2019–31. 1. 2020
2. Mgr. David Kubon, Charles University in Prague, Prague, Czech Republic, 30. 1.–5. 2. 2020
3. Dani Irawan, MSc, Technische Hochschule Köln, Köln, Germany, 1. 3.–15. 6. 2020
4. Mgr. David Kubon, Charles University in Prague, Prague, Czech Republic, 6.–12. 7. 2020
5. Gjorgjina Cenikj, Northern Macedonia, 1. 10.–31. 12. 2020
6. Iva Ivanov, Northern Macedonia, 1. 10.–31. 12. 2020

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1. Bojan Cestnik, Rebeka Kovačič Lukman, Andreja Abina, Andrej Flogie, Samo Repolusk, Maja Vičič Krabonja, Tanja Batkovič, Adem Kikaj, Ivan Boshkov, Nita Hasani, Maja Kurbus, Matevž Ogrinc, Jaka Progar, Nika Zagorc Okorn, Sabina Petek, Aleksander Zidanšek, "Development and implementation of a decision support expert system for monitoring sustainability-related competences at the secondary school", In: *15th SDEWES Conference, Conference on Sustainable Development of Energy, Water and Environment Systems, September 1-5, 2020, Cologne, Germany*, Proceedings, SDEWES, 2020, 0681.
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6. Gorjan Popovski, Gordana Ispirova, Nina Hadži-Kotarova, Eva Valenčič, Tome Eftimov, Barbara Koroušić-Seljak, "Food data integration by using heuristics based on lexical and semantic similarities", In: *BIOSTEC 2020, 13th International Joint Conference on Biomedical Engineering Systems and Technologies, February 24-26, 2020, Valletta, Malta*, Proceedings **1**: Biodevices, SciTePress, 2020, 208-216.
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PATENT

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DEPARTMENT OF KNOWLEDGE TECHNOLOGIES E-8

At the Department of Knowledge Technologies, we develop artificial-intelligence methods and advanced information technologies aimed at acquiring, storing and managing knowledge to be used in the context of the information- and knowledge-based society. Established areas of our work include machine learning (intelligent data analysis, data mining, and knowledge discovery in databases) and decision support, analysis of text and network data, language technologies, computational linguistics and digital humanities, as well as computational creativity and computational scientific discovery. In addition to performing research in knowledge technologies and methods, we also develop applications of such technologies in ecology and agriculture; bioinformatics, drug design, medicine, biomedicine, and ambient intelligence; economics, finance and marketing; and finally, space operations and Earth observation.

Head (until 31. 3. 2020):
Prof. Nada Lavrač

Head (since 1. 4. 2020):
Prof. Sašo Džeroski

In 2020 we were involved in 19 national projects, 13 Horizon 2020 projects (we acted as coordinators of two: EMBEDDIA and IMSyPP), two COST actions, one INTERREG V-A Slovenia-Italy project, two infrastructure projects, one smart specialization project, and five industry projects. The department hosted five junior researchers working towards their PhDs.

In the area of machine learning, we focused on **mining big and complex data**, developing various methods addressing different machine-learning tasks. First, we designed novel methods for feature ranking in the context of structured output prediction. We proposed and evaluated methods in the setting of supervised multi-label classification based on Relief and ensemble methods, as well as in the context of hierarchical multi-label classification. Moreover, we proposed a feature-importance estimation method using self-attention networks, and feature-importance estimation in the context of relational learning by using gradient boosting. Second, we developed and evaluated a methodology for estimating the quality of feature rankings. Third, we developed methods for learning option predictive clustering trees for multi-label classification and multi-target regression. Furthermore, we developed ensembles of extremely randomized predictive clustering trees for predicting structured outputs (the evaluation was performed in the context of multi-target regression, multi-label classification and hierarchical multi-label classification). We also developed multi-target regression rules with random output selection. Next, we extended the predictive clustering trees to consider multivariate splits in their nodes and evaluated them in the context of classification, and proposed to use hyperbolic embeddings for hierarchical, multi-label classification that improves the efficiency (and often the predictive performance) of predictive clustering trees and ensembles thereof. In the context of semi-supervised learning, we proposed a method for learning semi-supervised regression trees and applied it in the context of QSAR (Quantitative Structure–Activity Relationship), a method for learning regression trees from partially labelled data in the context of multi-target regression and considered its application for water quality assessment, and a method for incremental predictive clustering trees for online semi-supervised, multi-target regression.

Still in the context of **machine learning** and **intelligent data analysis**, data-mining methods for heterogeneous information network analysis were developed and used in several application domains. In the area of representation learning, we developed the SNoRE algorithm for the scalable unsupervised learning of symbolic node representations, published in *IEEE access*. The embedding-based Silhouette community detection algorithm was published in the *Machine Learning* journal. We also developed a new conceptual framework unifying two previously unrelated approaches, namely propositionalization and embeddings, and proposed two new algorithms combining the two approaches PropDRM and PropSpace, which we published in the *Machine Learning* journal.

Sašo Džeroski organized the online conference Space and AI, the first online conference on the space-related use of artificial intelligence (AI), on September 4, in conjunction with ECAI2020, the 24th European Conference on Artificial Intelligence (ECAI). With 5 keynotes, 17 contributed presentations and a panel discussion with 6 distinguished panellists, it attracted over 130 participants and was by far the largest of the over 60 side events of ECAI2020.

We have been also working on **semantic technologies** for supporting the process of data analysis in the spirit of open science. In particular, the IMPERATRIX project aims at improving the repeatability of experiments and the reusability of research outputs in complex data analysis. Within it, we worked on the further development of ontological descriptions of the domain of data analysis, as well as the development of a knowledge base, based on the developed ontologies. We extended the OntoDM-core ontology with a module for representing predictive modelling experiments as well as a module for representing multi-label classification methods. For the semantic annotation of predictive modelling datasets, we developed an annotation schema that contains entities for representing provenance information, the data type information as well as domain-specific information. In addition, we developed an annotation schema for the semantic annotation of predictive modelling experiments, which can be used for annotating different learning and validation scenarios. Finally, in the context of predictive modelling we developed a software system in the form of a web application that enables semantic annotation and the storage of different data-analysis entities and their storage in a triplet store through an end point. The stored triples can be queried using the SPARQL query language. Many of the above approaches produce models that are interpretable and can produce explanations of the predictions they make. In the context of explainable, trustworthy and human-centred artificial intelligence, two of our new projects are worth mentioning: the EU-funded project TAILOR, “Foundations of Trustworthy AI Integrating Learning, Optimisation and Reasoning” and the Slovenian project “Human Rights and Regulation of Trustworthy Artificial Intelligence”.

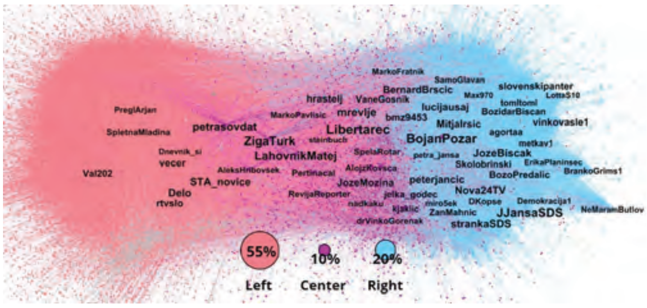

Figure 1: A Slovenian Retweet Network 2018-2020, coloured according to the detected communities. The legend shows the shares of total users in each of the three largest communities. The label size of a node corresponds to the number of unique users that have retweeted it. Only nodes with at least 700 unique retweeters are included. The community on the right is smaller and has more influential users, compared to the community on the left.

Besides the development of methods, we also consider many applications of machine learning in the context of **applied data science**, resulting in both publications and applied research and development projects. In the life sciences, we developed the CaNDis web server, which supports investigations of causal relationships between diseases, drugs, and drug targets, and was published in the prestigious *Bioinformatics* journal. We also developed an approach to multi-view clustering with mvReliefF for Parkinson’s disease patients subgroup detection and helped advance manufacturing systems by developing a novel conceptual framework for using big-data analytics in manufacturing. In the area of life sciences, medicine, pharmacology and nutrition, we developed the tool DietHub that analyses dietary habits through understanding the content of recipes, and used it to analyse changes in the food-consumption patterns of humans through the COVID-19 lockdown in the spring of 2020. Next, we performed a comprehensive empirical study of different molecular representations used in the task of predictive modelling. Furthermore, we developed a methodology for evaluating the quality of feature rankings and used it in biomarker discovery for embryonal tumours. In the context of biology and medicine, we proposed a predictive model for the quantitative analysis of human skin using photothermal radiometry and diffuse reflectance spectrometry; we discovered that distinct types of gut microbiota dysbiosis in hospitalized gastroenterological patients are disease non-related and characterized by predominance of either Enterobacteriaceae or Enterococcus; and we predicted associations between proteins and multiple diseases.

We worked on the SAAM H2020 project (Supporting Active Ageing through Multimodal Coaching), which aims to develop a virtual assistant-coach that supports the aging population living at home. Here we have continued the development of modelling and reasoning components of the coaching system, prepared the modules for sleep quality and cooking activity, and started testing them within the pilot testing phase. We have successfully finished the F4F project (Food 4 Future), where we have designed a methodology for distinguishing between natural and synthetic aromas and implemented it as a web application. In the scope of the H2020 project RESILOC (Resilient Europe and Societies by Innovating Local Communities), which aims at improving the resilience of local communities, we helped to define the knowledge representation and reasoning methodology and started to work on software components for the automatic detection of sentiment and trust in texts related to emergency and natural disaster response and mitigation procedures. Several applied research projects address the life sciences and medicine. We successfully completed the INTERREG V-A Slovenia-Italy project “TRAIN: Big Data and Disease Models: A Cross-border Platform for Validated Biotech Industry Kits”, where we developed machine-learning pipelines for virtual screening and drug repositioning. We successfully concluded our participation in the FET Flagship “Human Brain Project”, where we developed new data-mining methods and applied them to discover biological signatures of neuro-degenerative diseases. A novel method was developed for learning rule ensembles for multi-target regression, and applied it to analyse data on patients with Parkinson’s disease. Three national projects develop infrastructure, e.g., for bioinformatics (RI-SI ELIXIR), and use it on problems from life sciences, as well as to relate environmental exposure and human health. The latter is the topic of the project ”NEURODYS - Neuropsychological dysfunctions caused by low level exposure to selected environmental pollutants in susceptible population”, which looks at the effects of

Nada Lavrač and Sašo Džeroski organized a full-day seminar titled AI for Industry and Society, which took place at the Ljubljana Exhibition and Convention Center on February 12, 2020. With eight speakers from academia (four from our Department) and eight from Slovenian companies offering AI services, the event attracted over 100 participants.

exposure to mercury on the health of mothers and children. Another project in this area, "Restoration of moldy canvas paintings: improvement or deterioration?", concerns the damage to paintings caused by fungi. Finally, a cluster of projects and applied research looks 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 have also applied machine-learning methods (and in particular deep neural networks) to analyse remotely sensed data (and in particular the visualization of 3D LIDAR images) to classify Mayan architectural objects.

In the area of **decision support**, our long-term goal is to develop methods and techniques of decision modelling, support them with software and integrate them with data-mining systems. In addition to the TRUE project, presented below, we were involved in two decision-support-system development projects. In the first, EU H2020 project NARSIS, we developed a prototype system, called Severa, aimed at supporting severe accident management in nuclear power plants. So far, the system has been developed in full, and its extensive testing is planned for 2021. The second system, which is aimed at finding optimal tunnel routes, has been developed in the frame of the RRI 2 project TOPP, in collaboration with the companies Elea and XLab, and the JSI Department of Intelligent Systems (E9). We contributed a program module, called MAMo, that implements weight-based hierarchical models, specifically adapted for optimization. Additionally, the results of an already completed EU H2020 project PD_manager were published, presenting decision models for supporting medication-change decisions of Parkinson's disease patients. From the methodological and software perspective, our main contribution in 2020 is a new system DEX2Web (http://dex.ijs.si/). DEX2Web is a first web-based implementation of software supporting the DEX decision modelling method, which is heavily used in our projects. Substantial progress has also been achieved in "option generation", i.e., methods for investigating changes that can lead to an improvement or degradation of given decision alternatives. We designed and successfully verified a new approach based on Bayesian optimization, and presented it in an awarded conference paper.

Nada Lavrač gave a keynote talk titled "Semantic Relational Learning" at the 43rd German Conference on Artificial Intelligence, September 21–25, 2020 in Bamberg, Germany.

In the area of **knowledge technology applications in ecology and agriculture**, we are involved in several projects where we apply data-mining and decision-support methodologies for the development of predictive and decision-support models in the area of agronomy and systems ecology. Within the H2020 project TRUE (TRansition paths to sUstainable legume-based systems in Europe), we are developing a decision-support system for an assessment of the sustainability of the agri-food chains. In order to do that, we have taken into account three different sustainability aspects – environmental, social and economic. We assembled fifteen sustainability-assessment decision models into seven integrated models at three levels. All these models were integrated into a DSS system for an assessment of the overall sustainability of the entire agri-food chain - PathFinder - for which we have developed a graphical user interface. We developed a software class library, called TrueEval, which facilitates the use of integrated DEXi models in the context of the PathFinder DSS. The functionality, supported by the library, includes the inspection of DEXi models and their components, the evaluation of alternatives (agri-food chains) and the exploration of possibilities to improve or degrade a particular alternative. The system is being extensively tested by the project partners. The methodology used for the development of the system and decision models for an assessment of the sustainability of the agri-food chain were reported in the project deliverables. In the H2020 project TomRes (A novel and integrated approach to increase multiple and combined stress tolerance in plants using tomato as a model), we have two tasks. The first one deals with the prediction of resource-use efficiency of different tomato production systems using data-mining modelling. In the second task, we used expert knowledge, as well as knowledge obtained from the data-mining models (generated in the first task), to develop decision models that assess different tomato production systems with respect to environmental and socio-economic aspects. In both tasks, we were analysing two types of tomato-production systems: greenhouse and open-field production. The data-mining models were developed using experimental data from Greece and Mallorca. The decision models were developed to rank a set of decision alternatives (e.g., management or other activities in the tomato production) and choose the best one according to certain preferences. A model verification was performed to test their internal operational logic and behaviour. The domain experts used several well-known case studies as

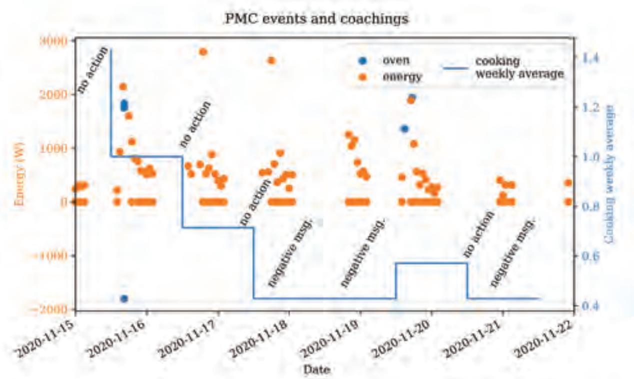

Figure 2: An overview of coaching messages (for one week) by the coaching system developed within the SAAM project. The system first uses a smart electricity meter (PMC) to detect the use of cooking appliances (blue dots) and other electricity consumers (orange dots). A set of decision models then assesses the situation (user's cooking activity has increased or decreased) and decides if a coaching message is needed (e.g., a negative message encouraging the user to cook more) or not (no action).

well as a theoretical one. The goal of the H2020 project IPM Decisions is to increase the impact of decision-support systems for integrated pest management (IPM). Within the project, our goal is to model the adoption of a DSS by potential users according to their profile and the type of IPM problems. To get a good understanding of the needs of DSS owners, developers and other potential users of the platform (farmers, advisors, researchers), workshops were organized in 12 project-partner countries at the beginning of 2020. We organized two workshops in Slovenia (one in Ljubljana and one in Maribor) with 40 participants in total. Through questionnaires, we gathered data about the preferences and barriers for the adoption of an IPM DSS platform. These data, together with the data from the workshops from the other 11 countries, were pre-processed and prepared for further analyses. The EUdaphobase COST Action aims to create the structures and procedures necessary for developing an open Europe-wide soil biodiversity data infrastructure. The ultimate goal of EUdaphobase is to establish a pan-European soil-biological data and knowledge warehouse, which can be used for understanding, protecting and sustainably managing soils, their biodiversity and functions. In this project, we are coordinating the working group where the key goals are to determine which results the assessment tools must offer to the stakeholders, to secure the corresponding data linkages within the data warehouse and to establish algorithms needed for developing the assessment tools. In 2020 we developed a conceptual framework for connecting the soil-data warehouse and the users using smart AI technologies.

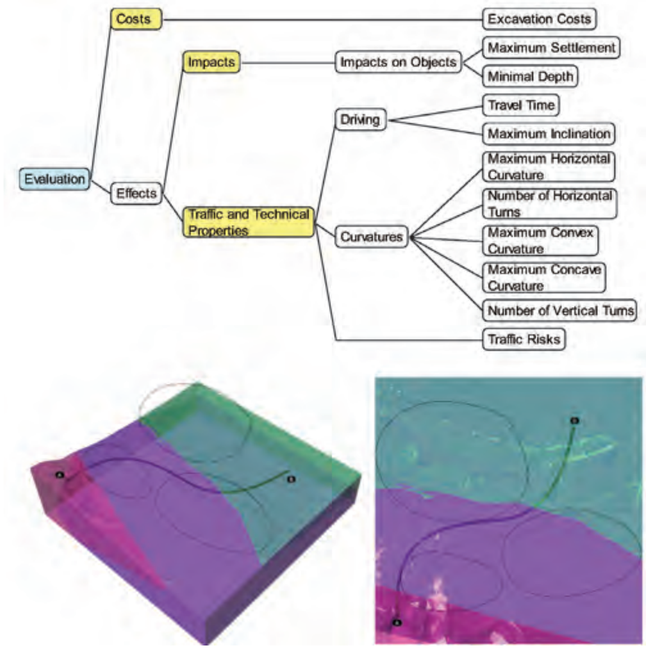

Figure 3: The structure of the decision model for evaluating tunnel routes, developed within the TOPP project (in cooperation with Elea iC d.o.o. and XLAB d.o.o.), and an example of a resulting optimal tunnel route considering different geological soil compositions (marked with different colours) and impact areas (marked with completed curves).

Concerning the use of **knowledge technologies in education**, we continued our collaboration with the University of Nova Gorica and JSI Center for Knowledge Transfer in IT. Our focus remained on the transformation of educational activities towards more flexible and open forms. Experimental analyses and investigations of the process itself were carried out in the context of higher education with the University of Nova Gorica as a test-bed. Although our work was carried out before the corona-virus epidemics, the situation after the publication has additionally proved its relevance. Together with the UNESCO chair in Open Technologies for Open Educational Resources and Open Learning at the JSI we continued to develop an innovative model of open education, which we are testing in practice in the Open Education for a Better World program (OE4BW). In particular, we focused on managing complexity, as hugely increased needs present new challenges to this field. Namely, the number of projects increased from 14 in 2018 to 110 projects accepted to be included in 2021. Newly introduced features such as topical hubs turned out to be very successful in practice. In December 2020 we contributed to the Pre-Expo online event where Slovenia presented its achievements in the field of Open Education, and the OE4BW program was featured as a good-practice example. Open Education Global, an international organization with about 200 institutional members from around the world, awarded the OE4BW program with the Open Collaboration Award for Excellence in 2020.

In the area of **text, web and network analysis** our research approach is to combine methods of text mining, network analysis and text analytics to reveal and highlight underlying characteristics in different domains. The main sources of data that we analyse are social media (Twitter, Facebook, YouTube), online news, annual financial reports, as well as other more structured data. We are coordinating a newly started EU project IMSyPP (Innovative Monitoring Systems and Prevention Policies of Online Hate Speech). The goal of the project is to develop models for automated hate-speech detection and tracking for four European languages (English, Italian, Slovene and Dutch). By applying the models to large datasets, we study hate-speech manifestations chronologically and geographically. So far, we have collected a large number of tweets in Slovene, and YouTube comments in Italian and English. The collected data were manually annotated for different levels of hate speech by multiple annotators, and first models for hate-speech classification were constructed by deep neural networks. We constructed and analysed the Slovenian re-tweet network in the period 2018–2020. The community-detection results show the prevalence of political discussions on Twitter and increasing polarization between the left- and right-leaning actors. Word embeddings represent words in a numeric space in such a way that semantic relations between words are encoded as distances and directions in the vector space. Cross-lingual word embeddings map the vector space of one language to the vector space of another language, or vector spaces of multiple languages to the joint vector space where similar

Petra Kralj Novak was a plenary speaker at the International School and Conference on Network Science 2020 as well as at the “Language Technology vs. Disinformation” workshop organized by DG CNECT of the European Commission.

words are aligned. Cross-lingual embeddings can be used to transfer machine-learning models between languages, thereby compensating for insufficient data in less-resourced languages. We use 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 did not increase the predictive performance. In collaboration with the University of Venice and a major Italian news outlet, Corriere della Sera, we measured the social response of users to different types of news framing. We analyse users' reactions in terms of toxicity, criticism of the newspaper, and stance concerning migration to posts on the newspaper's Facebook page and the corresponding news articles on the topic of migration. We found that visual pieces and factual news reports elicit the highest level of trust in the media source, while opinion pieces and editorials are more likely to be criticized. We also noticed that data-driven pieces elicit an extremely low level of trust in the news source. In machine learning, performance-estimation methods are used for assessing the generalization ability of predictive models. It is not always obvious which estimation method to employ to obtain the most realistic estimate of the errors that a predictive model will incur on unseen data. In our work we empirically evaluated the application of several methods to time-series forecasting tasks. We used 174 real-world time series and three synthetic time series. It turns out that the choice of the most appropriate estimation method depends on the stationarity or different sources of non-stationarity of the time series. In 2020 we started work on a new project FORMICA 2 (Quantitative and qualitative analysis of the unregulated corporate financial reporting). In preliminary work in the scope of this project we prepared a solution for the collection of forward-looking sentences from annual financial reports, which will be used in data sampling for development of datasets with financial sentiment annotations.

Department members participated in author profiling shared tasks within the scope of PAN, a series of scientific events and shared tasks on digital text forensics and stylometry. We ranked 3rd in Fake News spreaders profiling (out of 66 groups), and 2nd in celebrity profiling.

In the areas of **language technologies** and **digital humanities**, we work on methods to analyse text and on producing various types of language resources, with a focus on Slovene and other South Slavic languages. We continued our work on the European project EMBEDDIA (Cross-Lingual Embeddings for Less-Represented Languages in European News Media) that we coordinate. The EMBEDDIA project seeks to solve many problems for the news media industry in the analysis of news and comments, especially by leveraging innovations in the use of cross-lingual embeddings coupled with deep neural networks to allow existing monolingual resources to be used across languages. In 2020, we developed many new methods and applied them to various tasks, and organized a workshop on Natural language processing and digital humanities (collocated with PROPOR) and a shared task SemEval semantic evaluation workshop collocated with the COLING conference. We have developed several methods for addressing tasks of news-article classification. In the topic of sentiment analysis, we have addressed the task of zero-shot, cross-lingual, news-sentiment classification, where we used texts for training data only in Slovene, while the models can be applied to another language without any training data required. Further, we have evaluated various document-similarity methods for related news articles' recommendations. We have also focused on the development of methods for short-text classification. We have developed a novel approach tax2vec that leverages background knowledge from taxonomies to improve various short text classification tasks. Next, we have worked on news comment moderation (e.g., offensive speech detection), where we presented models trained on EMBEDDIA media partners' datasets in Croatian and Estonian. We have also participated in many shared tasks on author profiling and achieved 2nd place in Celebrity profiling, and 3rd place in the multilingual detection of fake-news spreaders, both organised in the scope of PAN@ CLEF. We have also published our paper from the GxG-CLIN29 shared task, which is one of the rare deep-learning solutions to author profiling. We have organised a shared task on predicting graded word similarity in the context in the scope of SemEval 2020, which represents a new natural language processing task that several international teams addressed in the scope of the competition. For this task, we developed a new resource CoSimLex, available through the CLARIN.SI research repository. Our novel methods for detecting semantic shift were evaluated in the scope of a shared task and were used for the diachronic news analysis in monolingual and multilingual settings.

Figure 4: Transition PathFinder - a DSS tool for the assessment of sustainability of the agri-food chain, according to the three sustainability pillars (environmental, social and economic) and their intersections (bearability, equitability and viability).

We continued work on the national research project FRENK "Resources, methods, and tools for the understanding, identification, and classification of various forms of socially unacceptable discourse in the information society" and on the Slovene-Flemish bilateral basic research project LiLaH "Linguistic landscape of hate speech on social media". We edited and wrote the introductory chapter of the book "The dark side of digital platforms: linguistic investigations of socially unacceptable online discourse practices" and investigated Twitter discourse on LGBTQ+ in Slovenia, water flow metaphors in Slovene online news migration discourse, Slovene socially unacceptable discourse on Facebook pages of news portals, as well as non-standard linguistic features, the grammatical footprint, and the use of demonstrative pronouns in Slovene socially unacceptable discourse on social media. We also published the LiLaH Emotion Lexicon of Croatian, Dutch and Slovene [http://hdl.handle.net/11356/1318]. We also co-organized three shared tasks. In the WMT shared task on translating similar languages we were responsible for the Slovene-Croatian and Slovene-Serbian translation pairs, and in the VarDial 2020 shared task on social media geolocation prediction, we were responsible for the Serbo-Croatian macro-language group. In the scope of the national project TERMFRAME, we have published a journal paper on replication and adaptation of a term-alignment approach, developed methods for mining terminological semantic relations using intersections of word embeddings, and presented a novel NetViz terminology visualization tool together with use cases in karstology domain modelling. In the scope of the European project SAAM, we have also addressed the task of emotion recognition from speech data, focusing on low-resource settings and automatic feature-selection methods, and a multimodal approach to the automated recognition of Alzheimer's dementia. We have also contributed to building and evaluating the resources for Slovene, including a reference list of Slovene common frequent words, and a comparison of different word-embeddings models in terms of gender bias. We published a synthetic paper on the results of the recently concluded national research project "Slovene scientific texts: resources and description", which produced a very large (1.5 billion word) annotated corpus of Slovenian diploma, masters and doctoral theses. We finalized and made available a large dataset of English-Slovene term candidates automatically extracted from the corpus of the project [http://hdl.handle.net/11356/1263], and performed a corpus-based analysis of the usage of epistemic modal adverbs in Slovenian academic discourse.

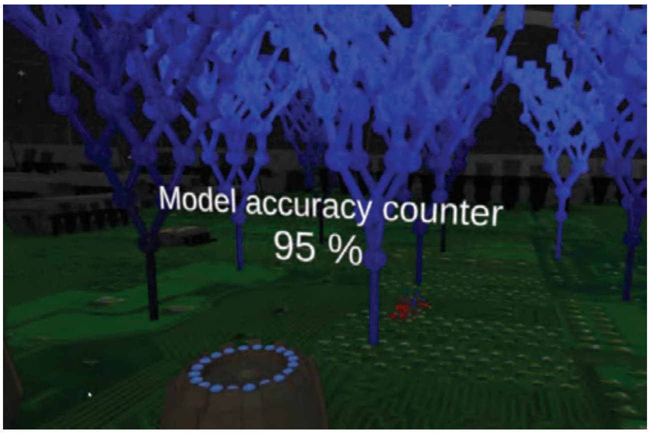

Figure 5: Within the TRAIN project, we developed virtual screening approaches for drug repositioning, as well as a virtual-reality representation of the process, including the machine learning of random forests.

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. In 2019, CLARIN.SI obtained a large grant for upgrading its computer cluster, and in 2020 we acquired and started using most of the cluster, and published a description of its current state and plans for the future. In 2020, the CLARIN.SI repository for language resources and tools was Core Trust Seal certified and its certification as a CLARIN ERIC Centre type B renewed. Fifty-one new resources were deposited into the repository, reaching a total of 202 resources at the end of the year. We contributed to the description of the main training corpus of Slovene, ssj500k and of the new version of the Slovene reference corpus Gigafida, to the development of a dataset for information spreading over the news and to a dataset for studying and analysing the complex event-outlet relationship. We also investigated how and how much language resources were cited in Slovenian scholarly publications in the period from 2013 to 2019. A new national project "Development of Slovenian in a Digital Environment" financed by the Slovenian Ministry of Culture and with partners from 12 institutions, started in 2020. The project aims to significantly extend language technologies and resources for Slovenian, with all the project resources that will be produced in the coming years to be archived and made available in the CLARIN.SI repository. CLARIN.SI will also offer 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. We have contributed to the field of digital humanities, by organising the Workshop on Digital Humanities and Natural Language Processing (DHandNLP 2020), co-located with International Conference on the Computational Processing of Portuguese (PROPOR 2020), where we also edited the conference proceedings volume, including our paper on word-embeddings-based analysis of Zofka Kveder's Work.

As part of the work of the CLARIN.SI and CLADA-BG Knowledge Centre for South Slavic languages (CLASSLA) [https://www.clarin.si/info/k-centre/] we either upgraded or made new models for various levels of linguistic annotation of standard and non-standard (social media) language for Slovenian [http://hdl.handle.net/11356/1312, http://hdl.handle.net/11356/1354, http://hdl.handle.net/11356/1325, http://hdl.handle.net/11356/1337, http://hdl.handle.net/11356/1350, http://hdl.handle.net/11356/1339], Croatian [http://hdl.handle.net/11356/1322, http://hdl.handle.net/11356/1331, http://hdl.handle.net/11356/1352, http://hdl.handle.net/11356/1340, http://hdl.handle.net/11356/1348, http://hdl.handle.net/11356/1357], Serbian [http://hdl.handle.net/11356/1349, http://hdl.handle.net/11356/1323, http://hdl.handle.net/11356/1332, http://hdl.handle.net/11356/1351, http://hdl.handle.net/11356/1341], Macedonian [http://hdl.handle.net/11356/1373, http://hdl.handle.net/11356/1374], and Bulgarian [http://hdl.handle.net/11356/1326, http://hdl.handle.net/11356/1328, http://hdl.handle.net/11356/1353, http://hdl.handle.net/11356/1329]. The freely available models can be used with the CLASSLA fork of the well-known StanfordNLP annotation tool-chain to annotate texts in these languages on the levels of morphosyntax, lemmatization, syntax, and named entities. We also produced the first word embeddings for Macedonian [http://hdl.handle.net/11356/1359] and a semantic hypergraph corpus for Croatian [http://hdl.handle.net/11356/1377]. The CLASSLA K-center furthermore extended its FAQ to cover, in addition to Slovene, Croatian and Serbian, also information on language resources and processing for Macedonian and Bulgarian, and organized, on 6th May 2020, a virtual workshop with 42 participants, which discussed future directions of language processing for South Slavic languages. CLARIN.SI was a co-organizer of the biennial Conference on Language Technologies and Digital Humanities [www.sdjt.si/jtdh-2020/], which took place virtually on the 24th and 25th September 2020. This international conference with a 22-year tradition is the main forum for the fields of language technologies and digital humanities in Slovenia, with the on-line proceedings for 2020 containing 28 contributions. We participated in the organization of the second ParlaCLARIN workshop with the title "Creating, Using and Linking of Parliamentary Corpora with other Types of Political Discourse". We co-edited the proceedings of the Workshop, co-authored the introduction, and presented our work - in cooperation with the Slovenian DARIAH infrastructure for the humanities - on the siParl corpus of Slovenian parliamentary debates, where we compiled and made available the second version of the siParl corpus, which contains carefully structured proceedings of the Slovenian parliament from 1990 to 2018 with over 200 million words. Based on the corpus, we wrote a tutorial that shows how corpora can be used to investigate language use and communication practices in a specialized socio-cultural context of political discourse. CLARIN.SI also became a partner in the 2020-2021 CLARIN ERIC funded project ParlaMint "Towards Comparable Parliamentary Corpora" where we cooperated in the compilation of the first version of the ParlaMint corpus, which contains linguistically annotated parliamentary proceedings 2015–2020 of Bulgaria, Croatia, Poland and Slovenia [http://hdl.handle.net/11356/1345]. At the CLARIN ERIC level, we participated in studies on creating a learner corpus infrastructure, on interoperability in an infrastructure enabling multidisciplinary research, on extending the CLARIN resource and tool families, on introducing the CLARIN European infrastructure, and on understanding and facilitating collaboration in Digital Humanities. We contributed to the work of the Slovenian Institute for Standardization as the Slovenian representatives in ISO/TC37/SC4 (Terminology and Other Language and Content Resources / Language Resources Management) by reviewing, translating and approving Slovenian standards from this field. We also continued to serve as technical editors for the on-line Slovenian Biographical Lexicon.

In the field of **computational creativity**, we have developed several methods using natural language processing techniques for creative scientific discovery. First, we presented lessons learnt on bisociative literature-based discovery, and developed a new word-embeddings approach that we applied in a setting of cross-domain discovery on biological texts. Next, we developed a method for COVID-19 therapy target discovery. Another contribution to the field of computational creativity is our analysis of the community publications in terms of reproducibility standards.

In the related field of **computational scientific discovery**, a key area of using artificial-intelligence methods for science, our research concentrated within the project SESAME - Automating the Synthesis and Analysis of Scientific Models. In the context of model synthesis, we developed methods for heuristic search through the space of process-based model structures, which perform well, are efficient and allow the exploration of larger spaces. In the context of model analysis, we explored the learning and use of surrogate models in several practical settings. This includes the use of complex simulation models of the response of human skin to light for diagnostic purposes, where we learn surrogate models that can be used for a very fast estimation of different skin parameters and properties. This also includes the learning of fast mappings from vectors of atmospheric parameters to shortwave infrared spectra for the Sentinel 5P satellite.

Some outstanding publications in the past year

1. Mileva Boshkoska, Biljana, Miljković, Dragana, Valmarska, Anita, Gatsios, Dimitros, Rigas, George, Konitsiotis, Spyros, Tsiouris, Kostas M., Fotiadis, Dimitrios I., Bohanec, Marko. Decision support for medication change of Parkinson's disease patients. Computer methods and programs in biomedicine. [Print ed.]. 2020, 35 pp. ISSN 0169-2607. DOI: 10.1016/j.cmpb.2020.105552.
2. Petković, Matej, Džeroski, Sašo, Kocev, Dragi. Multi-label feature ranking with ensemble methods. *Machine learning*. [Print ed.]. [in press] 2020, 19 pp. ISSN 0885-6125. DOI: 10.1007/s10994-020-05908-1.
3. Osojnik, Aljaž, Panov, Panče, Džeroski, Sašo. Incremental predictive clustering trees for online semi-supervised multi-target regression. Machine learning. [Print ed.]. 2020, vol. 109, no. 11, pp. 2121-2139. ISSN 0885-6125. DOI: 10.1007/s10994-020-05918-z.

4. Lavrač, Nada, Škrlj, Blaž, Robnik Šikonja, Marko. Propositionalization and embeddings: two sides of the same coin. *Machine learning*, ISSN 0885-6125. [Print ed.], 2020, vol. 109, no. 7, pp. 1465-1507, doi: 10.1007/s10994-020-05890-8.
5. Jean-Denis, Mathias, Debeljak, Marko, Trajanov, Aneta, et al. Grounding social foundations for Integrated Assessment Models of climate change: [commentary]. *Earth's future*. 2020, vol. 8, no. 7, 5 pp. ISSN 2328-4277. DOI: 10.1029/2020EF001573.

Awards and appointments

1. The paper "Generating alternatives for DEX models using Bayesian optimization", co-authored by Martin Gjoreski (E9), Vladimir Kuzmanovski (E8) and Marko Bohanec (E8), received the best paper award at the Slovenian Conference on Artificial Intelligence, SCAI 2020 (Ljubljana, 6.-7. October 2020).
2. Best lightning presentation award: B. Evkoski, I. Mozetič, N. Ljubešić, P. Kralj Novak. Evolution of political polarization on Slovenian Twitter, Complex Networks and their Applications, Madrid, Spain, December 1-3, 2020.
3. Boshko Koloski, Senja Pollak and Blaž Škrlj: Boshko Koloski, Senja Pollak and Blaž Škrlj: participation in the computer competition in the field of profiling of authors of PAN texts, where they achieved 2nd place in the field of profiling of celebrities (out of 66 groups) and 3rd place in the field of multilingual classification of users who share fake news

Organization of conferences, congresses and meetings

1. "Space and AI", first online conference on the use of artificial intelligence (AI) for applications in space technology. The conference was organized in association with the 24th European Conference on Artificial Intelligence ECAI, 4. 9. 2020 (virtual)
2. Organization of a full-day seminar entitled "Artificial Intelligence for Industry and Society", Gospodarsko razstavišče, Ljubljana, 12. 2. 2020.
3. SSHOC Webinar: CLARIN Hands-on Tutorial on Transcribing Interview Data, 3. 3. 2020 (virtual)
4. ParlaCLARIN II Workshop on Creating, Using and Linking Parliamentary Corpora with Other Types of Political Discourse, 11. 5. 2020 (virtual)
5. CLARIN Café I: CLARIN in times of Corona, 8. 6. 2020 (virtual)
6. CLARIN Café II: How to use CLARIN in (online) higher education, 10. 6. 2020 (virtual)
7. SSHOC Train-the-Trainer Bootcamp for Librarians, 22. 6. 2020 (virtual)
8. CLARIN Café III - CLARIN for Researchers: Literary Studies, 16. 7. 2020 (virtual)
9. Workshop Twin Talks 3: Understanding and Facilitating Collaboration in DH 23. 7. 2020 (virtual)
10. Conference on Language Technologies and Digital Humanities 2020, 24.–25. 9. 2020 (virtual)
11. CLARIN Annual Conference 2020, 5.– 7.10. 2020 (virtual)
12. Café@CLARIN2020: This is CLARIN. How Can We Help You?, 5. 10. 2020 (virtual)
13. Panel on Artificial Intelligence, Language Data and Research Infrastructures @ CLARIN2020, 7. 10. 2020 (virtual)
14. SSHOC Webinar: Sharing Datasets of Pathological Speech, 14. 10. 2020 (virtual)
15. Workshop Twin Talks 2: Understanding and Facilitating Collaboration in DH at DHN 2020 20.10.2020 (virtual)
16. CLARIN Café - Join Our Parliamentary-flavoured Coffee: ParlaMint, 3.11.2020 (virtual)
17. Seventh Workshop on NLP for Similar Languages, Varieties and Dialects VarDial2020, 13. 12. 2020 (virtual)
18. CLASSLA workshop, 6. –8. 5. 2020 (virtual)
19. Workshop on Digital Humanities and Natural Language Processing (DHandNLP 2020), co-located with International Conference on the Computational Processing of Portuguese (PROPOR 2020), Évora, Portugal 1. 4. 3. 2020

INTERNATIONAL PROJECTS

1. CLARIN Project ParlaMint - Towards Comparable Parliamentary Discourse
   Prof. Tomaž Erjavec
   Clarin Eric
2. COST CA16204; Distant Reading for European Literary History
   Prof. Tomaž Erjavec
   Cost Association Aisbl
3. COST CA18237; European Soil-Biology Data Warehouse for Soil Protection
   Prof. Marko Debeljak
   Cost Association Aisbl
4. H2020 - TRUE; Transition Paths to Sustainable Legume based Systems in Europe
   Prof. Marko Debeljak
   European Commission
5. 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
6. H2020 - NARSIS; New Approach to Reactor Safety Improvements
   Prof. Marko Bohanec
   European Commission
7. H2020 - SAAM; Supporting Active Ageing through Multimodal Coaching
   Asst. Prof. Bernard Ženko
   European Commission
8. H2020 - HBP SGA2; Human Brain Project Specific Grant Agreement 2
   Prof. Sašo Džeroski
   European Commission
9. H2020 - AI4EU; A European AI On Demand Platform and Ecosystem
   Prof. Sašo Džeroski
   European Commission
10. H2020 - RESILOC; Resilient Europe and Societies by Innovating Local Communities
    Dr. Aljaž Osojnik
    European Commission
11. H2020 - FNS-Cloud; Food Nutrition Security Cloud
    Prof. Nada Lavrač
    European Commission
12. H2020 - HECAT; Disruptive Technologies Supporting Labour Market Decision Making
    Asst. Prof. Biljana Mileva Boshkoska
    European Commission
13. H2020 - TAILOR; Foundations of Trustworthy AI - Integrating Reasoning, Learning and Optimization
    Prof. Sašo Džeroski
    European Commission
14. H2020 - ELEXIS; European Lexicographic Infrastructure
    Prof. Tomaž Erjavec
    European Commission
15. H2020 - EMBEDDIA: Cross-Lingual Embeddings for Less-Represented Languages in European News Media
    Asst. Prof. Senja Pollak
    European Commission
16. 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 inDialogue with Contemporary Use
   Prof. Tomaž Erjavec
5. CRISPR/CAS9-mediated targeted mutagenesis for resistance of grapevine and potatoagainst phytoplasmas
   Prof. Nada Lavrač
6. Resources, methods and tools for the understanding, identification and classification of various forms of socially unacceptable discourse in the information society
   Prof. Tomaž Erjavec
7. Semantic Data Mining for Linked Open Data Science
   Prof. Nada Lavrač
8. Improving Reproducibility of Experiments and Reusability of Research Outputs in Complex Data Analysis
   Asst. Prof. Pance Panov
9. Neuropsychological dysfunctions caused by low level exposure to selected environmental pollutants in susceptible population – NEURODYS
   Prof. Sašo Džeroski
10. Restoration of moldy canvas paintings: improvement or deterioration?
    Prof. Sašo Džeroski
11. Automating the Synthesis and Analysis of Scientific Models
    Prof. Sašo Džeroski
12. Predictive clustering on data streams
    Prof. Sašo Džeroski
13. Computer-assisted multilingual news discourse analysis with contextual embeddings
    Asst. Prof. Senja Pollak
14. Human Rights and Regulation of Trustworthy Artificial Inteligence
    Prof. Ljupčo Todorovski
15. Clinical course and outcome of Covid-19
    Prof. Sašo Džeroski
16. Food for future - F4F
    Asst. Prof. Bernard Ženko
    Ministry of Education, Science and Sport
17. TRAIN: Big Data and Disease Models: A Cross-border Platform for Validated Biotech Industry Kits
    Prof. Sašo Džeroski
    Ministry of Education, Science and Sport
18. Development of research Infrastructure for the international competitiveness of Slovenian RRI space - RI-SI ELIXIR
    Prof. Sašo Džeroski
    Ministry of Education, Science and Sport
19. Development of Slovene in the digital environment
    Prof. Tomaž Erjavec
    Ministry of Culture
20. Data Mining and Decision support in Sustainable Food Production
    Dr. Vladimir Kuzmanovski
    Ministry of Education, Science and Sport
21. Learning models of diseases and treatments for systems and personalized medicine
    Dr. Jovan Tanevski
    Ministry of Education, Science and Sport
22. 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. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
    Prof. Nada Lavrač
    Slovenian Research Agency

NEW CONTRACTS

1. Machine learning for Predicting Spacecraft Subsystem Power Consumption
   Prof. Sašo Džeroski
   Bias Variance Labs d. o. o.
2. AI4EO prototyping enviroment for Earth Observation
   Prof. Sašo Džeroski
   Bias Variance Labs d. o. o.
3. Multicriteria decision modeling for transparent tunnel design
   Asst. Prof. Bernard Ženko
   Elea Ic d. o. o.
4. Machine vision quality control of molded plastic parts
   Asst. Prof. Bernard Ženko
   Mpt, d. o. o.

VISITORS FROM ABROAD

1. Dr Gianvito Pio, KDDE Research Group @ Dept. of Computer Science, University of Bari Aldo Moro, Bari, Italy, 5. 2. 2020- 5. 8. 2020
2. Francesca Prisciandaro, KDDE Research Group @ Dept. of Computer Science, University of Bari Aldo Moro, Bari, Italy, 5. 2. 2020- 5. 8. 2020
3. Dr Ivica Dimitrovski, Faculty of Computer Science and Engineering, University of Skopje, North Macedonia, 5. –12. 2. 2020
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5. Michal Artur Szlupowicz, Warsaw University of Technology, Warsaw, Poland, 1. 7.–31. 8. 2020
6. Dr Richard Wheeler, The University of Edinburgh, Edinburg, Great Britain, 1. 9. 2020
7. Viktor Andonovikj, Ss. Cyril and Methodius University of Skopje, Skopje, North Macedonia, 1. 9.-30. 11. 2020
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52. Tina Anžič, B. Sc.

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BIBLIOGRAPHY

Original Article

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Short Article

1. Mathias Jean-Denis *et al.* (14 authors), "Grounding social foundations for Integrated Assessment Models of climate change: [commentary]", *Earth's future*, 2020, **8**, 7, e2020EF001573.

Published Conference Contribution

1. Bojan Cestnik, Rebeka Kovačič Lukman, Andreja Abina, Andrej Flogie, Samo Repolusk, Maja Vičič Krabonja, Tanja Batkovič, Adem Kikaj, Ivan Boshkov, Nita Hasani, Maja Kurbus, Matevž Ogrinc, Jaka Progar, Nika Zagorc Okorn, Sabina Petek, Aleksander Zidanšek, "Development and implementation of a decision support expert system for monitoring sustainability-related competences at the secondary school", V: *15th SDEWES Conference, Conference on Sustainable Development of Energy, Water and Environment Systems, September 1-5, 2020, Cologne, Germany*, Proceedings, SDEWES, 2020, 0681.
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15. Ana Kostovska, Sašo Džeroski, Panče Panov, "Semantic description of data mining datasets: an ontology-based annotation schema", In: *DS 2020, 23rd International Conference Discovery Science, October 19-21, 2020, Thessaloniki, Greece*, Proceedings, (Lecture notes in computer science **12323**), Springer, 2020, 140-155.
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17. Vedrana Vidulin, Sašo Džeroski, "Hierarchy decomposition pipeline: a toolbox for comparison of model induction algorithms on hierarchical multi-label classification problems", In: *DS 2020, 23rd International Conference Discovery Science, October 19-21, 2020, Thessaloniki, Greece*, Proceedings, (Lecture notes in computer science **12323**), Springer, 2020, 486-501.
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20. Matej Petković, Michelangelo Ceci, Kristian Kersting, Sašo Džeroski, "Estimating the importance of relational features by using gradient boosting", In: *ISMIS 2020, 25th International Symposium on Methodologies for Intelligent Systems, September 23-25, 2020, Graz, Austria*, Proceedings, Foundations of Intelligent Systems, (Lecture notes in computer science **12117**), Springer, 2020, 362-371.
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24. Miljenko Hojnić, Biljana Mileva Boshkoska, "A web-based decision support system for employee redeployment", In: *ICDSST 2020, 6th International Conference on Cognitive Decision Support Systems & Technologies, 27th-29th May, 2020, Zaragosa, Spain*, Proceedings, 2020, 228.
25. Marko Bohanec, Adem Kikaj, Ivan Vrbanić, Ivica Bašič, Klemen Debelak, Luka Štrubelj, "Supporting severe accident management in nuclear power plants", In: *ICDSST 2020, 6th International Conference on Cognitive Decision Support Systems & Technologies, 27th-29th May, 2020, Zaragosa, Spain*, Proceedings, 2020, 229.
26. Kristian Miok, Blaž Škrlj, Daniela Zaharie, Marko Robnik Šikonja, "Bayesian BERT for trustful hate speech detection", In: *ICML UDL 2020 Workshop on Uncertainty & Robustness in Deep Learning, July 17, 2020*, 2020.
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29. Matej Martinc, Senja Pollak, "Tackling the ADReSS challenge: a multimodal approach to the automated recognition of Alzheimer's dementia", In: *Interspeech 2020, 25-29 October, 2020, Shanghai, China*, Proceedings, ISCA online archive, 2020, 2157-2161.
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Independent Component Part or a Chapter in a Monograph

1. Kristina Pahor de Maiti, Darja Fišer, Nikola Ljubešić, "Hateful messages under linguist's scrutiny", In: *CMC Corpora through the prism of digital humanities*, (Collection Humanités numériques), L'Harmattan, 2020, 55-74.
2. Jennifer-Carmen Frey, Alexander König, Egon W. Stemle, Achille Falaise, Darja Fišer, Harald Lüngen, "The FAIR index of CMC corpora", In: *CMC Corpora through the prism of digital humanities*, (Collection Humanités numériques), L'Harmattan, 2020, 127-145.
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4. Vojko Gorjanc, Darja Fišer, "Twitter discourse on LGBTQ+ in Slovenia", In: *The dark side of digital platforms: linguistic investigations of socially unacceptable online discourse practices*, University Press, Ljubljana Faculty of Arts, 2020, 36-55.
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6. Ana Zwitter Vitez, "La contribution de la linguistique dans l'analyse de la dynamique sociale: l'exemple des Gilets jaunes", In: *Mikro in makro: pristopi in prispevki k humanističnim vedam ob dvajsetletnici UP Fakultete za humanistične študije*, Založba Univerze na Primorskem, 2020, 2, 509-526.
7. Donatella Gubiani, Irina Elena Cristea, Tanja Urbančič, "Introducing e-learning to a traditional university: a case-study", In: *Qualitative and quantitative models in socio-economic systems and social work*, Springer, 2020, 225-241.
8. Kristina Pahor de Maiti, Darja Fišer, Nikola Ljubešić, Tomaž Erjavec, "Analiza kazalnih zaimkov v družbeno nesprejemljivih spletnih komentarjih", In: *Slovenščina - diskurzi, zvrsti in jeziki med identiteto in funkcijo*, (Obdobja **39**), Znanstvena založba Filozofske fakultete, 2020, 89-99.

Scientific Monograph

1. Nataša Logar, Miha Grčar, Marko Brakus, Tomaž Erjavec, Špela Arhar Holdt, Simon Krek, *Korpusi slovenskega jezika Gigafida, KRES, ccGigafida in ccKres: gradnja, vsebina, uporaba*, Znanstvena založba Filozofske fakultete, 2020.

Theses and Mentoring

1. Stevanche Nikoloski, *Structured output prediction and modeling soil functions:* doctoral dissertation, Ljubljana, 2020 (mentor Sašo Džeroski; co-mentor David P. Wall).
2. Matej Petković, *Feature ranking for structured output prediction:* doctoral dissertation, Ljubljana, 2020 (mentor Sašo Džeroski; co-mentor Dragi Kocev).
3. Tomaž Stepišnik, *Complex nodes in trees for structured output prediction:* doctoral dissertation, Ljubljana, 2020 (mentor Dragi Kocev; co-mentor Sašo Džeroski).
4. Albert Zorko, *Modelling human cardiorespiratory system through heart-rate variability:* doctoral dissertation, Novo mesto, 2020 (mentor Zoran Levnajić; co-mentor Maximilian Moser).

DEPARTMENT OF INTELLIGENT SYSTEMS E-9

The Department of Intelligent Systems develops new methods and techniques for intelligent computer systems, with applications in the areas of the information society, computer science and informatics, and network communication systems. The main research areas are ambient intelligence, computational intelligence, agent and multi-agent systems, language and speech technologies, electronic and mobile health, and smart cities. The department 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 continuously 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 **CrowdHealth**, whose objective was to mine health data to help craft better public-health policies. The method for predicting physical stature, which we developed in the project in collaboration with the Faculty of Sports of the University of Ljubljana, is now being integrated into the SLOFit application. SLOfit is a national surveillance system for the physical and motor development of children and youth. The H2020 project **WellCo** created a virtual coach to advise older users on wellbeing and health. For this coach we developed methods to monitor nutrition with sensors and questionnaires, and to recognize the users' emotions from their voice. The H2020 project **Insension** is helping people with severe intellectual disability use digital services. We developed methods for the interpretation of their inner state using video from cameras and other sensors. In the Flemish-Slovenian project **STRAW**, whose objective is stress recognition from sensor data and analysis of stressors in the workplace, we started data collection with a sensing wristband and a mobile application. In the AAL project **CoachMyLife** we will help seniors with memory impairment perform everyday tasks. To this end, we developed methods to monitor nutrition and hydration with a sensing wristband and computer vision. We started the H2020 project **COVIRNA**, whose objective is to develop a diagnostic test for cardiovascular patients with COVID-19. We did other research on COVID-19, mainly a thorough analysis of factors affecting the spread of the disease in different countries using machine learning. We won an international **competition** on recognizing cooking activities from sensor data Cooking Activity Recognition Challenge. We also got to the second stage of the XPrize Pandemic Response Challenge, a competition in predicting COVID-19 infections and prescribing countermeasures (the competition continues in 2021). We finished **doctoral research** on methods for intelligently adjusting the operation of sensors to reduce energy consumption without sacrificing the sensing quality. We also finished doctoral research on the fusion of classical and deep machine learning for mobile health and behaviour monitoring with wearable sensors. We have ongoing doctoral research on the contact-free sensing of physiological signals and states.

We completed the project Multi-objective optimization for transparent tunnel design. The task was to design and implement a flexible method able to find a set of near-optimal tunnel routes where both the constraints and objectives for the route are chosen by the user.

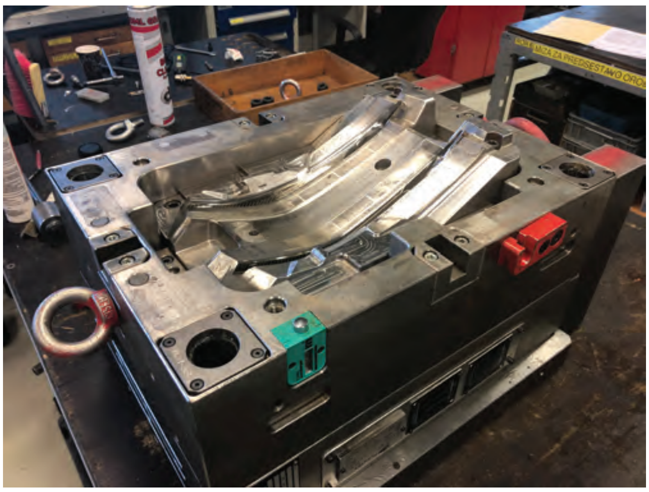

Figure 1: To improve the planning of tool manufacturing for injection molding, we developed a software solution to predict the duration of machining operations that relies on extracting features from 3D tool drawings and machine learning of predictions based on these features.

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 smart homes, and intelligent healthcare support systems. This consists of developing new algorithms, methods and approaches by introducing artificial intelligence into computer systems. In 2020 we started a series of new projects. In the Interreg Italy-Slovenia programme, we

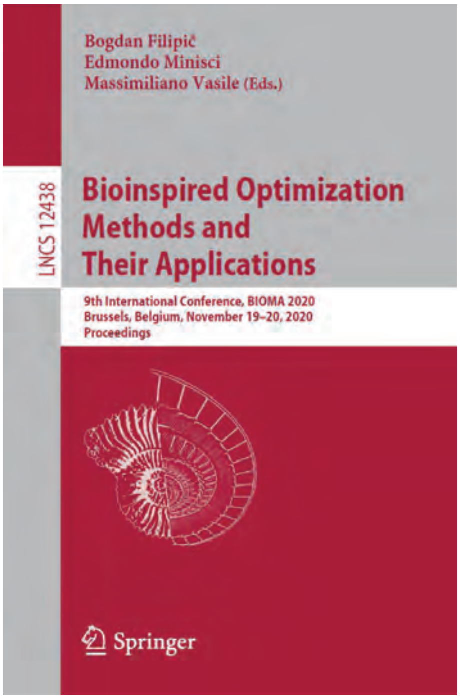

Figure 2: We coorganized the 9th International Conference on Bioinspired Optimization Methods and Their Applications, BIOMA 2020, that was held virtually on 19-20 November 2020. The conference proceedings were published by Springer in the series Lecture Notes in Computer Science.

launched the **Insieme** project, which is developing a platform for electronic and mobile health (EMH), which will offer 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 a number of new and innovative devices and solutions to support elderly and chronic patients at home, where, among other things, we already developed a smartwatch for the elderly, but we are now transferring it to mobile phones. In addition to 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, to warn of the risk of falling. For the **H2020 Urbanite smart cities** project, we developed a first prototype of a system that simulates traffic in Bilbao. The project includes four European cities: Amsterdam, Helsinki, Bilbao and Messina. The system will ultimately enable city managers to validate and identify the best mobility policies and measures. As part of the European **ERA PerMed BATMAN** project, where the theme is the Acne Inversa disease research, we developed a prototype that enables data input, display and processing. Partners-physicians from European countries will be able to enter data on patients in order to create a sufficiently large database for processing using AI methods. In the framework of the **ROBKONCEL** project, in cooperation with Gorenje and Unior, we developed a prototype of an intelligent system for comprehensive quality control in production with a reconfigurable robotic control cell and an intelligent process-control system. For the company **Comland**, we developed an intelligent system for managing the application in natural language. For the company **NiceLabel** we developed a system for intelligent webmail sorting, which determines the scope based on content and helps in creating responses.

Computational intelligence is a study of stochastic search, optimization and learning methods, inspired by biological and physical systems. Research in this area at the Department of Intelligent Systems focuses on evolutionary computation and optimization. We study evolutionary algorithms for multi-objective optimization, their acceleration through parallel computing and surrogate models, constraint handling in multi-objective optimization, visualization of optimization results, methodology of algorithm benchmarking, and their applicability in science and engineering. In 2020, we completed several industrial projects based on this expertise. In collaboration with the INEA company, we developed **a computer system to schedule flexible offers for electricity production and consumption** aimed at reducing the mismatch between the available and the needed electrical energy. The system uses mixed-integer linear programming as an optimization methodology. Testing at several pilot installation sites in various European countries showed the system is capable of producing high-quality schedules of flexible offers under strict time requirements. We also completed the project **Multi-objective optimization for transparent tunnel design** for the XLAB company. The task was to design and implement a flexible method able to find a set of near-optimal tunnel routes where both the constraints and objectives for the route are chosen by the user. We solved this task by encoding tunnel routes with clothoids and using a multi-objective evolutionary algorithm to find trade-off solutions. This method proved to be efficient in solving problems with objectives as diverse as minimal costs, best technical characteristics and minimal environmental impacts. Finally, we participated in two **Key Enabling Technologies for Clean Production (KET4CP)** projects for small manufacturing enterprises Plamtex INT and MPT. The first project was devoted to the improved planning of tool manufacturing for injection moulding where the task was to predict the duration of machining operations needed to manufacture the tools, and the developed solution relies on extracting features from 3D tool drawings and the machine learning of predictions based on these features. The goal of the second project was to design a machine-vision system to monitor the quality of moulded plastic products, and our role was to construct models for classifying the products into quality classes and assess their accuracy.

We used machine learning to perform probably the most thorough analysis to date of factors affecting the spread of COVID-19 in different countries. We focused on the early period before countermeasures overshadowed other factors.

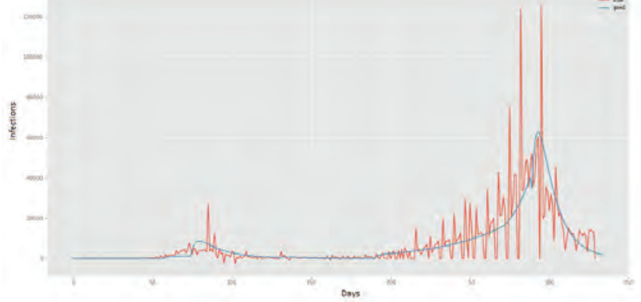

Figure 3: We participated in the "XPRIZE: Pandemic response challenge" competition, where we were tasked with estimating the number of COVID-19 infections. In the figure we show our prediction for France, for the year 2020, compared to the actual infection values.

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/). Its fourth version was released this year. The synthesizer is improved in terms of both comprehensibility and natural perception of the speech. A new high-quality female voice was added. 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 since this year. We also developed a service of speech synthesis for mobile devices (http://dis.ijs.si/dyslex/), which is free for anyone to use. We completed successfully the CityVOICE project: "Speech Technologies with Advanced Language Resources". We continue to work on the AudiBook project: "Education accessibility through a digital audio library for the blind and visually impaired".

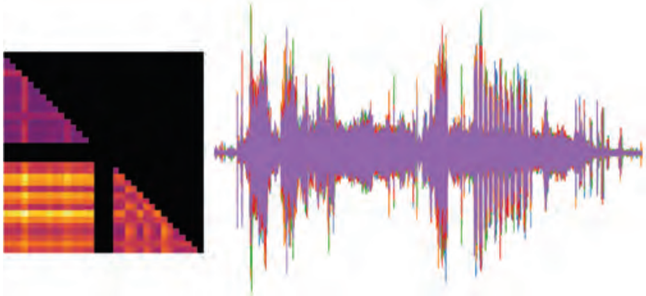

Figure 4: We implemented a tool-wear assessment based on sensor data from a production process. The figure shows a comparison of vibrations at the initial treatments (i.e., after tool replacement) with the vibrations at the final treatments (i.e. before the next tool replacement).

The **23rd International Multiconference Information Society – IS 2020** (is.ijs.si) took place at the Jožef Stefan Institute from October 5 to 9, 2020. It consisted of 8 independent conferences with 160 presentations. Four conference awards were presented: for lifetime achievements ("Donald Michie and Alan Turing" award) to prof. dr. Lidija Zadnik Stirn, for current achievements in the field of information society to the ACM Bober Competition Program Committee, and the information strawberry (Laboratory for Bioinformatics, Faculty of Computer and Information Science, University of Ljubljana) and lemon (unresponsiveness in the development of the electronic health record) for the best and worst public information-society services.

Figure 5: In 2020, the 23rd International Multiconference Information Society – IS 2020 (is.ijs.si) consisted of eight separate conferences. Four awards were handed out, of which the Lifetime Achievement Award (recognition of "Donald Michie and Alan Turing") was presented to Prof. Dr. Lidija Zadnik Stirn.

Together with the University of Strathclyde we organized the 9th International **Conference on Bioinspired Optimization Methods and Their Applications (BIOMA 2020)** that was held virtually on 19-20 November 2020. BIOMA is a conference series providing an opportunity for the research community in bio-inspired optimization to present recent achievements and discuss new ideas in the field. This year the conference programme consisted of the invited talks by Prof. Gabriela Ochoa on recent advances in local optima and search trajectory networks and Prof. Enrique Alba on algorithms for smart cities, and 24 presentations of regular papers. The conference proceedings were published by Springer in the series Lecture Notes in Computer Science (LNCS).

Some outstanding publications in the past year

1. Gjoreski, M., Janko, V., Slapničar, G., Mlakar, M., Reščič, N., Bizjak, J., Drobnič, V., Marinko, M., Mlakar, N., Luštrek, M., Gams, M. Classical and deep learning methods for recognizing human activities and modes of transportation with smartphone sensors. Information Fusion, 2020, **62**, 47-62.
2. Álvarez-García, J. A., Cvetković, B., Luštrek, M. A survey on energy expenditure estimation using wearable devices. ACM Computing Surveys, 2020, **53** (5), 1-35.
3. Gjoreski, M., Gradišek, A., Budna, B., Gams, M., Poglajen, G. Machine learning and end-to-end deep learning for the detection of chronic heart failure from heart sounds. IEEE Access, 2020, **8**, 20313-20324.
4. Varelas, K., El Hara, O. A., Brockhoff, D., Hansen, N., Manh Nguyen, D., Tušar, T., Auger, A. Benchmarking large-scale continuous optimizers: The bbob-largescale testbed, a COCO software guide and beyond. Applied Soft Computing, 2020, **97**, part A, 106737-1–106737-13
5. Zupančič, J., Filipič, B., Gams, M. Genetic-programming-based multi-objective optimization of strategies for home energy-management systems. Energy, 2020, **203**, 117769-1–117769-15

Awards and appointments

1. Stefan Kalabakov, Simon Stankoski, Nina Reščič, Andrejaana Andova, Ivana Kiprijanovska, Vito Janko, Martin Gjoreski, Mitja Luštrek: SHL Challenge – Sussex-Huawei Locomotion and Transportation Recognition Challenge, 3rd Place Award, virtual, Dr Hristijan Gjoreski, University of Sussex (UK) & Ss. Cyril and Methodius University (MK), Dr Lin Wang, University of Sussex (UK), Prof. Daniel Roggen, University of Sussex (UK), Dr Kazuya Murao, Ritsumeikan University (JP), Dr. Tsuyoshi Okita, Kyushu Institute of

Technology (JP), Mathias Ciliberto, University of Sussex (UK), Paula Lago, Kyushu Institute of Technology (JP), method for recognition of locomotion activity from smartphone sensors

2. Clément Picard, Vito Janko, Nina Reščič, Martin Gjoreski, Mitja Luštrek: The Cooking Activity Recognition Challenge 1st Place Award, virtual / Kitakyushu, Japan, ABC Conference, method for recognition of cooking activities with sensors
3. Maj Smerkol: Best paper award at People and Environment, 23rd International Multiconference Information Society, IS 2020, Ljubljana, Jožef Stefan Institute, Traffic Simulation Software in the Context of Mobility Policy Support System
4. Tea Tušar: Best Paper award at Human-Computer Interaction in Information Society, 23rd International Multiconference Information Society, IS 2020, Ljubljana, Jožef Stefan Institute, Interactive visualization of the Slovenian budget with the Sankey diagram

Organization of conferences, congresses and meetings

1. 36th Slovenian Workshop on Nature-Inspired Algorithms, AVN, Maribor, 29 September 2020 (virtual)
2. 9th International Conference on Bioinspired Optimization Methods and Their Applications, BIOMA 2020, Brussels, Belgium, 19–20 November 2020 (virtual)
3. 37th Slovenian Workshop on Nature-Inspired Algorithms, AVN, Ljubljana, 2 December 2020 (virtual)
4. UbiTtention 2020: 5th International Workshop on Smart & Ambient Notification and Attention Management, UbiComp 2020, Cancun, Mexico, 12 September 2020 (virtual)
5. Slovenian Conference on Artificial Intelligence 2020 (subconference of the 23rd International Multiconference Information Society (IS 2020)), Ljubljana, 6–7 October 2020
6. 23rd international multiconference Information Society, IS2020, Ljubljana, 5–9 October 2020
7. GECCO Job Market at the Genetic and Evolutionary Computation Conference, GECCO 2020, Cancun, Mexico, 10 July 2020 (virtual)
8. On-Body Sensor Networks workshop (OBSN 2020) at the International Conference on Embedded Wireless Systems and Networks (EWSN 2020), Lyon, France, 17 February 2020
9. 23. International Multiconference, IS 2020, Ljubljana, 5–9 October 2020, independent conferences:
   - Professional Ethics
   - Human-Computer Interaction in Information Society
   - Data Mining and Data Warehouses
   - Cognitive Science
   - People and Environment
   - International Technology Transfer Conference
   - Slovenian Conference on Artificial Intelligence
   - Education in Information Society

Patents granted

1. Alexander Gilenson, Boštjan Kaluža, Oz Eyal, System and method for automated detection of anomalies in the values of configuration item parameters, US10635557 (B2), US Patent Office, 28. 04. 2020.
2. Alexander Gilenson, Boštjan Kaluža, Oz Eyal, System and method for incident root cause analysis, US10691522 (B2), US Patent Office, 23. 06. 2020.

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. COST CA17129: CardioRNA - Catalysing Transcriptomics Research in Cardiovascular Disease
   Dr. Mitja Luštrek
   Cost Association Aisbl
3. H2020 - CrowdHEALTH; Collective Wisdom Driving Public Health Policies
   Dr. Mitja Luštrek
   European Commission
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. Development of AI Methods for Monitoring Affective States Using Unobtrusive Sensors
   Prof. Matjaž Gams
   Slovenian Research Agency

10. 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. Disentangling the sources and context of daily work stress: a comprehensive real-time modelling study using wearbles and technological detections
   Dr. Mitja Luštrek
2. Food for future - F4F
   Dr. Mitja Luštrek
   Ministry of Education, Science and Sport
3. Italian-Slovenian Ecosystem for Electronic and Mobile Health
   Prof. Matjaž Gams
   Regione Autonoma Friuli Venezia Giulia, Direzione
4. SI4CARE
   Dr. Mitja Luštrek
   Ministry of Economic Development and Technology
5. CoachMyLife
   Dr. Mitja Luštrek
   Ministry of Public Administration
6. ML-Aml: Application og Machine Learning Methods to Ambient Intelligence: Psychsocial Stress and Beahviour analysis
   Prof. Matjaž Gams
   Public Scholarship, Development, Disability and Maintenance Fund of the Republic of Slovenia
7. BATMAN: Biomolecular Analyses for Tailored Medicine in Acne iNversa
   Prof. Matjaž Gams
   Ministry of Education, Science and Sport
8. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
   Prof. Matjaž Gams
   Slovenian Research Agency
9. 23nd International Multiconference Information Society 2020, IS 2020, Ljubljana, Slovenia, 5 October 2020 - 9 October 2020
   Prof. Matjaž Gams
10. CLD - Cognitive Load Dataset
    Dr. Mitja Luštrek
    Fraunhofer-Institut für Integrierte

VISITOR FROM ABROAD

1. Prof. dr Boris Naujoks, Beate Breiderhoff, Cologne University of Applied Sciences (TH Köln), Gummersbach, Germany, 9–11 March 2020

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36. Blaž Mahnič, B. Sc.
37. Nina Reščič, B. Sc.
38. *Marjetka Šprah, B. Sc., left 01.09.20*
39. Lana Zemljak

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ORIGINAL ARTICLE

1. Juan Antonio Álvarez-García, Božidara Cvetković, Mitja Luštrek, "A survey on energy expenditure estimation using wearable devices", *ACM computing surveys*, 2020, **53**, 5, 91.
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4. Konstantinos Varelas, Ouassim Ait El Hara, Dimo Brockhoff, Nikolaus Hansen, Duc Manh Nguyen, Tea Tušar, Anne Auger, "Benchmarking large-scale continuous optimizers: the bbob-largescale testbed, a COCO software guide and beyond", *Applied soft computing*, 2020, **97**, a, 106737.
5. Luka Pirker, Anton Gradišek, Bojana Višić, Maja Remškar, "Nanoparticle exposure due to pyrotechnics during a football match", *Atmospheric environment*, 2020, **233**, 117567.
6. Jana Krivec, Matej Guid, "The influence of context on information processing", *Cognitive processing*, 2020, **21**, 2, 167-184.
7. Jernej Zupančič, Bogdan Filipič, Matjaž Gams, "Genetic-programming-based multi-objective optimization of strategies for home energy-management systems", *Energy*, 2020, **203**, 117769.

8. Martin Gjoreski, Anton Gradišek, Borut Budna, Matjaž Gams, Gregor Poglajen, "Machine learning and end-to-end deep learning for the detection of chronic heart failure from heart sounds", *IEEE access*, 2020, **8**, 20313-20324.
9. Martin Gjoreski, Matjaž Gams, Mitja Luštrek, Pelin Genc, Jens-U. Garbas, Teena Hassan, "Machine learning and end-to-end deep learning for monitoring driver distractions from physiological and visual signals", *IEEE access*, 2020, **8**, 70590-70603.
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1. Tine Kolenik, Matjaž Gams, "Progressing social good by reducing mental health care inequality with persuasive technology", In: *Harvard CRCS Workshop AI for social good, July 20-21, 2020*, Proceedings, 2020.
2. Aljoša Vodopija, Vito Janko, Mitja Luštrek, Bogdan Filipič, "Constrained multiobjective optimization for the design of energy-efficient context recognition systems", In: *BIOMA 2020, Bioinspired optimization methods and their applications, 9th International Conference, November 19-20, 2020, Brussels, Belgium*, Proceedings, (Lecture notes in computer science **12438**), Springer, 2020, 308-320.
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5. Matjaž Gams, "Izumiranje Slovencev in drugih narodov", In: *Okrogla miza kadrovska vrzel v Sloveniji: zakaj v Sloveniji primanjkuje ljudi v delovni starosti, 30. januar 2020, Ljubljana*, zbornik, Inštitut dr. Antona Korošca, 2020, 30-32.
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7. Carlo De Masi, Mitja Luštrek, "Drinking detection from videos in a home environment", In: *Slovenian Conference on Artificial Intelligence, 6-7 October 2020, Ljubljana, Slovenia*, Proceedings of the 23rd International Multiconference Information Society (IS 2020), volume A, Institut "Jožef Stefan", 2020, 15-18.
8. Erik Dovgan, Bogdan Filipič, "Semantic feature selection for AI-based estimation of operation durations in individualized tool manufacturing", In: *Slovenian Conference on Artificial Intelligence, 6-7 October 2020, Ljubljana, Slovenia*, Proceedings of the 23rd International Multiconference Information Society (IS 2020), volume A, Institut "Jožef Stefan", 2020, 19-22.
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17. Tine Kolenik, Matjaž Gams, "Increasing equality (in mental health care) with persuasive technology", In: *Slovenian Conference on Artificial Intelligence, 6-7 October 2020, Ljubljana, Slovenia*, Proceedings of the 23rd International Multiconference Information Society (IS 2020), volume A, Institut "Jožef Stefan", 2020, 55-58.
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27. Matjaž Gams, "Etika in mediji", In: *Professional Ethics, 7 October, 2020, Ljubljana, Slovenia*, Proceedings of the 23rd International Multiconference Information Society (IS 2020), volume D, Institut "Jožef Stefan", 2020, 8-11.
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31. Jernej Zupančič, Miha Štravs, Miha Mlakar, "MightyFields Voice: voice-based mobile application interaction", In: *Human-Computer Interaction in Information Society, 9 October 2020, Ljubljana, Slovenia*, Proceedings of the 23rd International Multiconference Information Society (IS 2020), volume H, Institut "Jožef Stefan", 2020, 13-16.
32. Jerneja Žganec Gros, Miro Romih, Tomaž Šef, "eBralec 4: hibridni sintetizator slovenskega govora", In: *Human-Computer Interaction in Information Society, 9 October 2020, Ljubljana, Slovenia*, Proceedings of the 23rd International Multiconference Information Society (IS 2020), volume H, Institut "Jožef Stefan", 2020, 17-20.
33. Tine Kolenik, Martin Gjoreski, Matjaž Gams, "Designing an intelligent cognitive assistant as persuasive technology for stress, anxiety and depression relief", In: *PERSUASIVE-ADJ 2020, 15th International Conference on Persuasive Technology Adjunct, April 20th - 23rd, 2020, Aalborg, Denmark*, Proceedings, (CEUR workshop proceedings **2629**), CEUR, 2020, poster 6.
34. Stefan Kalabakov, Simon Stankoski, Nina Reščič, Ivana Kiprijanovska, Andrejaana Andova, Clement Picard, Vito Janko, Martin Gjoreski, Mitja Luštrek, "Tackling the SHL challenge 2020 with person-specific classifiers and semi-supervised learning", In: *UbiComp/ISWC '20 adjunct, the 2020 ACM International Joint Conference on Pervasive and Ubiquitous Computing and the 2020 ACM International Symposium on Wearable Computers, September 12-17, 2020*, Proceedings, ACM, 2020, 323-328.

Independent Component Part or a Chapter in a Monograph

1. Hristijan Gjoreski, Simon Stankoski, Ivana Kiprijanovska, Anastasija Nikolovska, Natasha Mladenovska, Marija Trajanoska, Bojana Velichkovska, Martin Gjoreski, Mitja Luštrek, Matjaž Gams, "Wearable sensors data-fusion and machine-learning method for fall detection and activity recognition", In: *Challenges and trends in multimodal fall detection for healthcare*, (Studies in systems, decision and control **273**), Springer, 2020, 80-96.
2. Hernan Aguirre, Tanaka Kiyoshi, Tea Tušar, Bogdan Filipič, "Optimization and visualization in many-objective space trajectory design", In: *High-performance simulation-based optimization*, (Studies in computational intelligence **833**), Springer, 2020, 93-112.
3. Jörg Stork, Martina Friese, Martin Zaefferer, Thomas Bartz-Beielstein, Andreas Fischbach, Beate Breiderhoff, Boris Naujoks, Tea Tušar, "Open issues in surrogate-assisted optimization", In: *High-performance simulation-based optimization*, (Studies in computational intelligence **833**), Springer, 2020, 225-244.
4. Jana Krivec, Primož Rakovec, Tjaša Stepišnik Perdih, "The role of ICT in adolescents dealing with psychosocial problems", In: *Technology and social choices in the era of social transformations*, P. Lang, 2020, 59-79.

Scientific Monograph

1. Andrej Raspor, Metka Nežič, Nevenka Podgornik, Jana Krivec, Primož Rakovec, Bojan Macuh, Miha Černetič, Kaja Kos, Vanja Tajnšek, Marija Turnšek Mikačić, Irena Kopitar, Maja Ptičar, MilošPožar, *S skrbjo za sodelavce do boljših rezultatov podjetja*, Perfectus, 2020.

Professional Monograph

1. Lina Boljka *et al.* (37 authors), *Bela knjiga o strokovnem varovanju okolja*, Institut "Jožef Stefan", 2020.

Patent

1. Alexander Gilenson, Boštjan Kaluža, Oz Eyal, *System and method for automated detection of anomalies in the values of configuration item parameters*, US10635557 (B2), US Patent Office, 28. 04. 2020.
2. Alexander Gilenson, Boštjan Kaluža, Oz Eyal, *System and method for incident root cause analysis*, US10691522 (B2), US Patent Office, 23. 06. 2020.

Theses and Mentoring

1. Martin Gjoreski, *A fusion of classical and deep machine learning for mobile health and behavior monitoring with wearable sensors:* doctoral dissertation, Ljubljana, 2020 (mentor Matjaž Gams; co-mentor Mitja Luštrek).

DEPARTMENT OF REACTOR ENGINEERING

R-4

The Department of Reactor Engineering is involved in basic and applied research in the fields of nuclear engineering and safety. Topics include theoretical and experimental research of basic thermal-hydrodynamic phenomena, thermal-hydraulic safety analyses of fission and fusion reactors, structural safety analyses and probabilistic safety assessment. 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 in undergraduate and doctoral studies programmes. In 2020, using knowledge from nuclear energy, the department was also involved in the modelling of the development of the COVID-19 epidemic in Slovenia

Head:
Prof. Leon Cizelj

Modelling of basic thermal-hydrodynamic phenomena

In the frame of two-phase, gas-liquid flow research, we simulated a Taylor bubble 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 a Large Eddy Simulation (LES), which allows a high-fidelity reproduction of the flow. The results were validated using measurements obtained in our own THELMA laboratory. The simulations overestimate the Taylor bubble's decay rate by about one-to-two orders of magnitude, which shows that the bubble's break-up mechanism is severely overestimated.

The basic phenomena of vapour explosion, which might occur during a hypothetical severe accident at a nuclear power plant (NPP) if the hot reactor-core melt comes into contact with the coolant, were investigated. Studies of vapour explosions in stratified melt-coolant configurations were continued. The developed mechanistic model of the premixing layer formation, based on theoretical research and recent experiments, was implemented into the MC3D code (Institut de radioprotection et de sûreté nucléaire - IRSN, France), and validated with experimental results.

The potential for vapour explosions during a core melt-sodium interaction was also further investigated. The simulations of sodium vapour explosion were performed using the MC3D code in potential experimental conditions. The sensitivity study results in selected geometries that indicate that the pressure loads of the vapour explosion in sodium are lower than in water. Furthermore, we proposed a modification of the dimensionless Biot number for assessing the importance of the melt's thermal conductivity on the melt fragments quenching.

In the field of hydrogen distribution in NPP containment, simulations of atmosphere stratification erosion using a vertical jet, performed in the PANDA facility (Paul Scherrer Institute - PSI, Switzerland) were continued. We also participated in benchmark simulations of an experiment on stratified atmosphere erosion using natural convection, performed in the THAI+ facility (Becker Technologies, Germany), where we used the ASTEC system code (IRSN). For such scenarios, we also proposed a methodology for scaling up the results, obtained on experimental facilities, to real plants.

In the field of hydrogen combustion, we used the ASTEC code as well to participate in the simulation benchmark of two combustion experiments, performed in the ENACCEF II facility (Centre national de la recherche scientifique, France), within the project SAMHYCO-NET.

We used the ANSYS CFX CFD code to simulate an experiment on reactor core melt behaviour in the reactor pressure vessel lower plenum, performed on the LIVE2D experimental facility (Karlsruhe Institute of Technology, Germany).

Experimental investigations in the THELMA laboratory

Turbulent temperature fluctuations on a heated foil in a liquid flow were observed with an infra-red camera.

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 nuclear reactor fuel assembly. Following tests in the horizontal rod position, the first tests were also performed in the vertical position. In order to close the thermal balances, measurements were performed in the single-phase flow regime. These measurements were used for the validation of a CFD model of the entire test section that includes the inlet and outlet legs. The heat transfer inside the apparatus was studied using a series of CFD simulations for different cases where the primary and secondary fluid are isothermal as well as non-isothermal. In the two-phase flow regime, nucleate boiling was observed with a fast camera and the obtained images were post-processed using in-house-developed software, which provides data on the void distribution around the rods.

The Taylor bubble experimental facility was modified in order to achieve larger flow rates, better flow control, illumination and image quality. A custom-designed glass box was installed around the transparent test section, which successfully reduced the optical distortions of the recorded light. Measurements of the Taylor bubble decay rate were obtained and used for the validation of the Taylor bubble simulations in the counter-current flow regime (as described at the beginning).

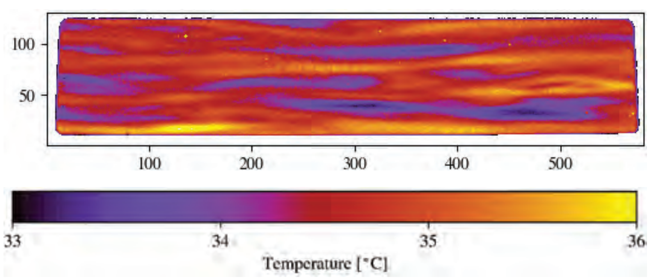

Figure 1: Instantaneous temperature field on a heated foil in a liquid flow.

As modelling of turbulent heat transfer behind a backward-facing step with spectral-element-based Direct Numerical Simulation (DNS) produced an accurate description of the flow field, a new test section of plexiglass was used for a detailed measurement of the velocity field, without heat transfer, which were performed in water using the Particle Image Velocimetry technique and compared with simulations. The same phenomenon was modelled with the wall-resolved LES-WALE turbulence model. Despite an accurate turbulence model, there are slight but distinct differences between the average flow fields observed in DNS and LES computations.

In a newly constructed experimental loop, a fully developed turbulent flow in a rectangular duct was heated with a thin metal foil powered with DC current. Temperature turbulent fluctuations were observed on the outer side of the foil using an infrared camera. In parallel with the measurements, a LES model of the considered phenomenon was developed, which successfully predicted the outcome of the measurements, including the power spectra of the temperature fluctuations on the heated foil.

Thermal-hydraulic safety analyses of fission and fusion reactors

After the accident at the Fukushima-Daiichi NPP in Japan in 2011, design extension conditions (DEC) were introduced in Europe as the preferred method for giving due consideration to complex sequences as well as severe accidents. The LP-FW-01 test, which falls within the DEC and was performed in 1983 on the Loss of Fluid Test Facility (Idaho National Engineering Laboratory, USA), represents a fault sequence in which a total loss of feedwater to the steam generator is followed by recovery using primary system feed-and-bleed. The test was simulated with the RELAP5/MOD3.3 computer code. The short-term simulation results match the major events of the test very well, whereas in the long term simulation, the liquid entrainment to the surge line is important for the correct prediction.

We were the first to perform an accurate simulation of the temperature distribution in the breeding blanket inside a fusion reactor during its remote replacement.

The European project PIACE considers the concept of a passive isolation condenser, which is suitable for automatic limitation of the reactor core's cooling rate during an accident. For water-cooled reactors, the concept is suitable for preventing thermal shocks in the vessel and piping walls. Experiments on a reduced scale will be performed in the SIRIO facility (SIET, Italy). We have performed a scaling-down analysis and proposed suitable experimental conditions, as well as a necessary modification of the facility, for an experiment related to pressurized-water-reactor technology.

The thermal loading of the DEMO fusion reactor breeding blanket (BB) during the remote maintenance operation and ex-vessel loss-of-coolant accident was analysed considering the decay heat generated inside the BB in the frame of the European nuclear fusion project WPPMI. Transient simulations were performed to evaluate the cooling performance and temperature distribution of passive, in-vessel components due to in-vessel air natural convection. The CFD simulations are supported with the results of a lumped-parameter model, which was used for fast predictions of longer transients.

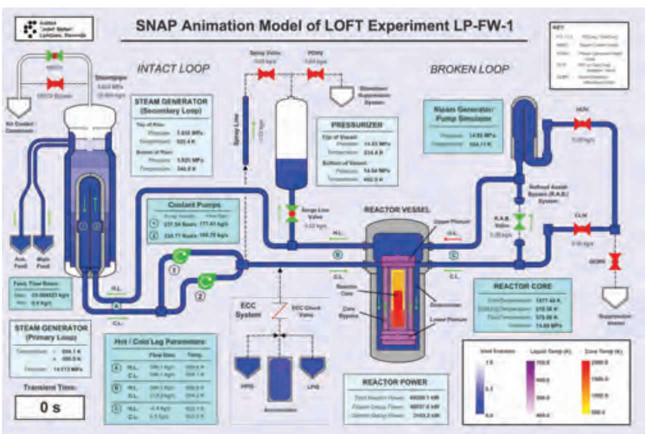

Figure 2: Animation model of Loss of Fluid Test Facility (INEL, USA).

A new reciprocating probe was developed for plasma diagnostics in European fusion tokamaks in the frame of the European fusion project WP-MST2. The probe design has to undergo a number of tests (theoretical and experimental) before it can be used in an actual tokamak. In this respect, the probe's resilience to the heat loads in the AUG (ASDEX Upgrade) tokamak in Germany was studied numerically. The predicted thermal response of the probe to the typical plasma discharge experiment in AUG has shown the need for a thicker protective shroud, with a 2-mm increase being sufficient.

We continued with the development of 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 design is based on the expected beam power distribution of DTT NBI, thermal-hydraulic parameters (limiting temperatures of the structure and coolant, pressure drop) and geometrical constraints. Realistic temperature distributions over the entire panel were determined using a two-step procedure: in the first step, a detailed numerical simulation using a coupled fluid-solid approach was performed on a reduced model; in the second step, the extrapolated heat-transfer coefficient was used to calculate the temperatures over the entire panel. The work was performed in collaboration with Consorzio RFX (Italy).

Structural safety analyses

A micromechanical analysis of the intergranular stress corrosion cracking of an irradiated austenitic stainless steel was performed in cooperation with Commissariat à l'énergie atomique et aux energies alternatives (CEA, France) to assess local cracking conditions. Micromechanical simulations based on a reconstructed 3D microstructure rationalized the correlation obtained experimentally into a single stress-based criterion.

The effect of different grain-boundary types on intergranular normal stresses was studied in a polycrystalline material (also in cooperation with CEA). A new parameter was identified, which is able to solely quantify normal stress fluctuations on a particular grain-boundary type.

A micromechanical analysis of intergranular stress-corrosion cracking of an irradiated austenitic stainless steel was performed to assess local cracking conditions.

A strategy for the efficient use of high-resolution CFD results in fatigue analyses of pipes is being developed within the European project ATLAS+, with the goal to perform thermo-mechanical analyses with arbitrary finite-element meshes. Fracture-mechanics models of a cracked pipe were developed for the subsequent crack-growth analyses using both CFD and stochastic temperature fields.

In pressurized thermal shock studies, the cooperation with PSI continued as fracture-mechanics analyses of an embrittled reactor pressure vessel were carried out in 1D and 3D models using uniform and non-uniform cooling conditions, respectively. Review activities related to state-of-the-art methods and national experience on pressurized thermal shock were initiated within the European project APAL.

Thermo-mechanical analyses of a dry cask for nuclear spent-fuel storage were performed in the framework of the cooperation with the Polytechnic University of Madrid (Spain).

We also participated in three European fusion projects. In WPDC (diagnostic and control), a feasibility study of the thermo-current measurement in the isolated-target divertor model in the DEMO fusion reactor was performed. The structural integrity of the cooling pipes during an extreme plasma disruption event was investigated for variable pipe-cassette contact resistivity.

Thermo-mechanical analyses were performed to evaluate the deformations and stresses of the calorimeter's conceptual design for the DTT NBI. Finally, the thermo-mechanical response of a new diagnostic probe inside the ASDEX Upgrade tokamak was analysed.

Probabilistic safety assessment

The purpose of a probabilistic safety assessment (PSA) is the quantification of risk in complex industrial systems. The European NARSIS project aims to extend the present PSA methodologies to extreme events with very low frequencies. In 2020, we dealt with constraining uncertainty in the event of a long-term station blackout. We first considered parameters that influence a probabilistic safety analysis the most. We then assessed the effect of parameter changes (diesel generator operating time, type of coolant loss, core cooling delay and pressure drop) using the fast-Fourier-transform-based method by signal mirroring (FFTBM-SM), which mostly influence and can change qualitatively the course of events, which is further addressed by probabilistic safety analysis.

Modelling of COVID-19 epidemic development in Slovenia

We have developed a SEIR (Susceptible, Exposed, Infectious, Recovered) type model with extensions for forecasting the progression of an epidemic, which reduces all the complexity of the epidemic to the behaviour of a single point, which represents the entire country. The equations for the spread of infections are similar to the equations of the chain reaction in a nuclear reactor. With the model, which was fitted with publicly available data, the impact of the population's response to the measures taken to contain the epidemic can also be taken into account.

For the government expert advisory group, we have been preparing daily analyses of the epidemic situation and prognoses of the number of hospitalized people.

In the model, we consider in an integral way most of the available data, such as: daily and cumulative number of confirmed cases, daily, current and cumulative number of people hospitalized and in intensive-care units, daily and cumulative number of deceased people, and their age structures. Immunisation and vaccination are also taken into account. We consider separately homes for the elderly and the rest of Slovenia, and infections introduced from

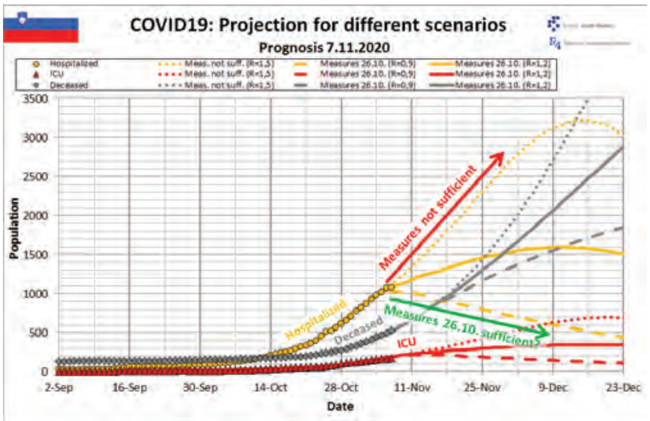

Figure 3: Projection of number of hospitalized COVID-19 patients in ordinary and intensive-care units and cumulative number of deceased for different scenarios of epidemic development.

abroad. We treat four different courses of the disease in comparison and calculate nine specific reproductive numbers of the spread of the infection, on the basis of which the trend of the epidemic is determined. We check the initial part of the prognosis with what we already have 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, appear in hospitals, intensive-care units and finally die. We also take into account soft data, i.e., information that is not provided in the form of numbers, 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 expert advisory group, we prepared daily analyses of the epidemic situation and prognoses of the number of hospitalized (separately for intensive-care units) and deceased people, and an estimate of the reproductive number of infections R (which must be below one to contain the epidemic), based on which the impact of measures on R can be assessed. The results of our analyses and the prognoses were regularly published on the public website of our department.

Technical cooperation, consulting services and education

In 2020 the Reactor Engineering Division cooperated in a project for industry as well. As an authorized institution for radiation and nuclear safety, we prepared an independent evaluation of the changes in the licencing documentation of the Krško nuclear power plant related to the containment isolation and reactor trip signals.

Researchers of the department represent the core staff of the Chair for Nuclear Engineering at the Faculty of Mathematics and Physics at the University of Ljubljana, and are involved in nuclear engineering undergraduate, master and doctoral studies. The programmes are associated with the European Nuclear Education Network (ENEN). In the school year 2020/21, the first students of the international MSc program in nuclear engineering SARENA, in which the department is actively involved, were admitted to the Faculty of Mathematics and Physics.

Awards and appointments

1. Julio Benavides, Oriol Costa Garrido, Gonzalo Jimenez, Leon Cizelj: Best poster award (NENE2020 conference, Portorož) Nuclear Society of Slovenia, Thermo-mechanical Analysis of a Dry Storage System
2. Jan Kren, Dean's Award for Outstanding Academic Achievement UL FMF, University of Ljubljana
3. Rok Krpan, Best Video Presentation–European Award (International conference ICONE 2020, virtual) American Society of Mechanical Engineers, Simulations of Experiments on Isothermal Containment Atmosphere Mixing Caused by Vertical Injection

Patent granted

1. Marko Matkovič, Iztok Tiselj, Ivo Kljenak, Andrej Prošek, Matjaž Leskovar, Ljubo Fabjan, Leon Cizelj, Method and apparatus for assessing the state of spent-fuel facility, GB2530969 (B), UK Patent Office, 08. 04. 2020.

INTERNATIONAL PROJECTS

1. CROSSING - Crossing Borders and Scales - An Interdisciplinary Approach
   Dr. Boštjan Končar
   Helmholtz-zentrum Dresden-rossendorf E.v.
2. Training and Tutoring for Experts of the National Regulatory Authorities and their Technical Support Organisations for Developing or Strengthening their Regulatory and Technical Capabilities - MC3.01/13
   Prof. Leon Cizelj
   Iter-consult Srl - Independent
3. H2020 - ATLASplus; Advanced Structural Integrity Assessment Tools for Safe Long Term Operation
   Prof. Leon Cizelj
   European Commission
4. H2020 - NARSIS; New Approach to Reactor Safety Improvements
   Dr. Andrej Prošek
   European Commission
5. H2020 - ENENplus; Attract, Retain and Develop New Nuclear Talents Beyond Academic Curricula
   Asst. Prof. Ivo Kljenak
   European Commission
6. H2020 - PIACE; Passive Isolation Condenser
   Asst. Prof. Ivo Kljenak
   European Commission
7. H2020 - sCO2-4-NPP; Innovative sCO2-Based Heat Removal Technology for an Increased Level of Safety of Nuclear Power Plants
   Dr. Andrej Prošek
   European Commission
8. H2020 - EURAD; European Joint Programme on Radioactive Waste Management
   Prof. Leon Cizelj
   European Commission
9. H2020 - ECC-SMART; Joint European Canadian Chinese Development of Small Modular Reactor Technology
   Prof. Leon Cizelj
   European Commission
10. H2020 - AMHYCO; Towards an Enhanced Accident Management of the Hydrogen/CO Combustion Risk

Asst. Prof. Ivo Kljenak
European Commission
11. H2020 - APAL; Advanced PTS Analysis for LTO
Dr. Oriol Costa Garrido
European Commission
12. H2020 - EUROfusion; Research Unit - Administration and Services RU – FU
Dr. Boštjan Končar
European Commission
13. H2020 - EUROfusion; Education-ED-FU
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14. H2020 - EUROfusion; Plant Level System Engineering-PMI-PPPT-FU
Dr. Boštjan Končar
European Commission
15. H2020 - EUROfusion; Diagnostic and Control-WPDC-PPPT-FU
Dr. Boštjan Končar
European Commission
16. H2020 - EUROfusion; Preparation and Exploitation of Medium Size Tokamaks - WPMST2-FU
Dr. Boštjan Končar
European Commission
17. H2020 - EUROfusion; WPSAE-PPPT-FU, WP27
Dr. Boštjan Končar
European Commission

RESEARCH PROGRAMMES

1. Reactor engineering
Prof. Leon Cizelj
2. Fusion technologies
Dr. Boštjan Končar

R&D GRANTS AND CONTRACTS

1. Pressurization process during vapour explosion in sodium cooled fast reactors
Dr. Mitja Uršič
2. Efficient cooling concepts for high heat flux components in fusion reactor
Dr. Boštjan Končar
3. Investigation of turbulent heat transfer in an annulus through advanced experimental and computational methods
Prof. Iztok Tiselj
4. Simulation of selected design extension conditions without core melt
Dr. Boštjan Končar
5. Understanding stratified steam explosions in reactor conditions
Dr. Matjaž Leskovar
6. Reimbursement of costs of scientific publications in golden open access for 2019, 2020
Prof. Leon Cizelj

NEW CONTRACT

1. The challenges of long term operation of Krško NPP beyond 40 years
Dr. Martin Draksler
Ministry of the Environment and Spatial Planning

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1. Marko Matkovič, Iztok Tiselj, Ivo Kljenak, Andrej Prošek, Matjaž Leskovar, Ljubo Fabjan, Leon Cizelj, *Method and apparatus for assessing the state of spent-fuel facility*, GB2530969 (B), UK Patent Office, 8. 04. 2020.

REACTOR INFRASTRUCTURE CENTRE RIC

The Reactor Infrastructure Centre (RIC) incorporates a TRIGA Mark II research reactor and a Hot Cells Facility. The reactor, which has been operating since 1966, is used for neutron research, education and training, as well as radioactive isotope production. A detailed technical description of the reactor is available at http://www.rcp.ijs.si/~ric/. The Hot Cells Facility is used for the treatment and handling of radioactive materials and radioactive waste, for both research and applicative projects. In addition, it is used for performing regular radiological measurements of radioactive waste and irradiated samples.

Members of the reactor staff operate and maintain the reactor. They also participate in other activities, requiring specialists skilled in working with sources of radiation and in reactor technology, such as 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 2020 the reactor operated for 126 days (464 hours) and produced 78.8 MWh of heat. Altogether, 37 pulses were carried out and 952 samples were irradiated in the irradiation channels. The reactor operated less than in the previous years, due to the Covid-19 pandemic. We didn't reject any offers, and yet, the demand for the reactor facilities was not as high as usual. Therefore, we reached only 70% of produced energy in comparison to 2019, but we managed to surpass the number of irradiated samples.

The reactor 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 2020 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 also 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

The reactor was used for the following research activities:

- Reactor physics and neutronics.
- Activation analysis.
- Research on 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.

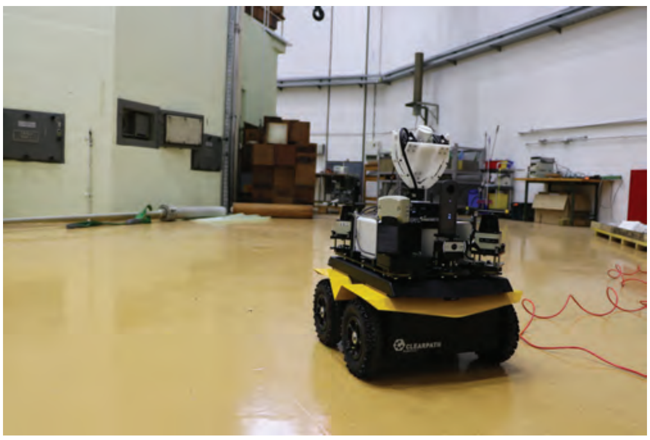

Figure 1: Testing of an autonomous vehicle designed for dose-rate field mapping.

In January a cycle of practical classes for master's students at the Faculty of Mathematics and Physics, University of Ljubljana was completed.

The same cycle of practical classes begun again in October; this time with a different approach, as it was mostly carried out remotely.

In January, in collaboration with the University of Lancaster, the effectiveness of an autonomous robot that can measure both gamma and neutron dose fields was tested. Our collaboration extended to the area of glycol and glycerine transmutation.

In February the damaged reactor-building window panes were replaced with new ones.

Figure 2: In September, the Reactor Physics Department (F8) and the Reactor Infrastructure Centre (RIC) personnel carried out the first remote reactor-physics course. Students at the University of Uppsala were able to follow the reactor activities and staff lectures via the Zoom platform.

In March the practical part of training for the future staff of Krško NPP started.

In April, sterilization tests for the FFP2 and FFP3 protective masks were performed.

In June and July the practical training for the future Krško NPP staff was resumed. Some exercises were conducted remotely, while others were completed in normal circumstances.

Our collaboration with Rolls-Royce Civil Nuclear SAS (Meylan, France) continued into 2020. Two campaigns were carried out, one in June and the second one in November. Their main purpose was the development of nuclear instrumentation.

In August, FT-TIMS samples were irradiated for CEA (mass spectrometry with the help of thermal ionization).

In September the Reactor Physics Department (F8) and the Reactor Infrastructure Centre (RIC) personnel carried out the first remote reactor physics course. Students at the University of Uppsala were able to follow the reactor activities and staff lectures via the Zoom platform. We also provided management of our experimental equipment. The students could gather our reactor's data and process it in Sweden.

In December, a campaign of pulse-mode operation was performed. Its purpose was to test the response of a Cherenkov radiation detector.

Throughout the year, many samples for CERN and other large particle accelerators were irradiated, in collaboration with the Department of Experimental Particle Physics (F9), or directly for the contractor.

In June 2019 the Jožef Stefan Institute signed an agreement with the European Commission, Directorate-General for Research and Innovation, Fission Energy *"Grant Agreement Number 847555",* together with the project coordinator - *Slovenska Technicka Univerzita v Bratislave (Slovak University of Technology in Bratislava)* and other institutions, namely with *Technische Universitaet Wien (Vienna University of Technology),* Česke *Vysoke Uceni Technicke v Praze (The Czech Technical University in Prague) and Budapesti Muszaki es Gazdasagtudomanyi Egyetem (The Budapest University of Technology and Economics).* The project is called ENEEP – EUROPEAN NUCLEAR EXPERIMENTAL EDUCATIONAL PLATFORM, and its purpose is to create a European-level platform that would provide experimental and educational activities in the field of nuclear science and technology for students and young professionals. The project that started together with the Reactor Physics Department (F8) continued into 2020. In 2020 our department and the F8 department collaborated mostly on WP3, its purpose being gathering information on experimental devices and equipment, educational activities, potential users, and SWOT analyses. The work on WP4 began, which we coordinate, to pursue activities that will eventually establish the platform itself.

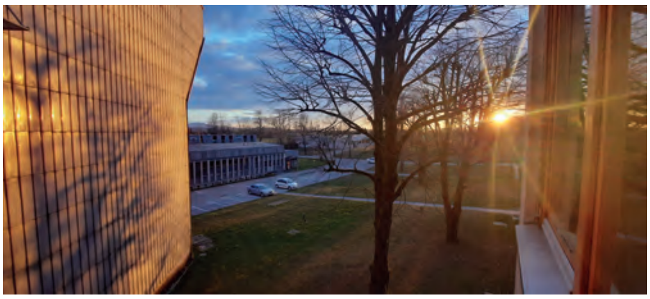

Figure 3: TRIGA Reactor at sunset.

Collaboration with the company DITO, which develops and sells the best radiation-resistant lighting, continued in 2020. Specific lighting components were irradiated to decide their levels of radiation hardness.

The reactor operators participated in the replacement of radioactive sources (C0-60 and Cs-137) for the Laboratory for Dosimetry Standards, operating under the Department of Low and Medium Energy Physics (F2).

To stop the spread of the new coronavirus, the number of visitors at the reactor was strictly limited. Open day at JSI, where the reactor usually participates, was cancelled. However, the Reactor Infrastructure Centre took part in the event called European Researchers' Night, where visitors could take a virtual walk around the reactor. Due to positive feedback, a video was recorded in collaboration with the Nuclear Training Centre, enabling virtual visits to the reactor for all Slovenian students.

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. Irradiation of Glycol
   Dr. Anže Jazbec
   Lancaster University
3. Irradiations on the TRIGA Reactor
   Prof. Borut Smodiš
4. Irradiation of FT-TIMS Samples
   Dr. Anže Jazbec
   CEA - Commissariat A L' Energie Atomique
5. Irradiation and Analysis of Samples in the Year 2019 - Part II
   Dr. Anže Jazbec
   National Nuclear Research Center
6. Irradiations of FT-TIMS Capsule on the TRIGA Reactor for Years 2020-2022
   Prof. Borut Smodiš
   Cea - Commissariat A L' Energie Atomique Et Aux
7. Refubrished Lazy Susan
   Prof. Borut Smodiš
   University Of Pavia
8. Sample irradiation using technology for determination of neutron and gama dose
   Prof. Borut Smodiš
   Ministry of Agriculture, Forestry and Food

NEW CONTRACT

1. Treatment and conditioning of radioactive waste for storage
   Prof. Borut Smodiš
   ARAO

VISITORS FROM ABROAD

1. Januar Ioannis Tsitsimpelis, Chris Tighe, Andrew West, Lancaster University, United Kingdom, 27 January 2020 – 31 January 2020
2. Clement Barnier, Seremie Durand, Stephane Fargues, Rolls Royce Civil Nuclear S.A.S, Meylan, France, 22 June 2020 – 24 June 2020
3. Gaël De Cargouët, Pierre Vignollet, Clemente Barnier and Stephane Fargues, Rolls Royce Civil Nuclear S.A.S, Meylan, France, 16 November 2020 – 19 November 2020

STAFF

Researcher
1. **Prof. Borut Smodiš, Head**

Postgraduate
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 (invited lecture)

1. Luka Snoj *et al.* (22 authors), "Radiation hardness studies and detector characterisation at the JSI TRIGA reactor", In: *ANIMMA 2019, Advancements in Nuclear Instrumentation Measurement Methods and their Applications, June 17-21, 2019, Portorož, Slovenia*, Proceedings, (EPJ Web of Conferences **225**), EDP Sciences, 2020, 04031.

Published Conference Contribution

1. Andrej Žohar, Anže Pungerčič, Klemen Ambrožič, Vladimir Radulović, Anže Jazbec, Sebastjan Rupnik, Igor Lengar, Luka Snoj, "Conceptual design of irradiation facility with 6 MeV and 7 MeV gamma rays at the JSI TRIGA Mark II research reactor", In: *ANIMMA 2019, Advancements in Nuclear Instrumentation Measurement Methods and their Applications, June 17-21, 2019, Portorož, Slovenia*, Proceedings, (EPJ Web of Conferences **225**), EDP Sciences, 2020, 04014.
2. Igor Lengar, Sebastjan Rupnik, Andrej Žohar, Vid Merljak, Marjan Kromar, Luka Snoj, "Usage of multiple fission cells for neutron flux measurements during rod-insertion method", In: *ANIMMA 2019, Advancements in Nuclear Instrumentation Measurement Methods and their Applications, June 17-21, 2019, Portorož, Slovenia*, Proceedings, (EPJ Web of Conferences **225**), EDP Sciences, 2020, 04024.
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7. Anže Jazbec, Sebastjan Rupnik, Vladimir Radulović, Jan Malec, Andraž Verdir, Marko Rosman, Borut Smodiš, Luka Snoj, "Jožef Stefan Institute TRIGA research reactor activities in the period from September 2019 - August 2020", In: *NENE 2020, 29th International Conference Nuclear Energy for New Europe, September 7-10, Portorož, Slovenia*, Proceedings, Nuclear Society of Slovenia, 2020, 304.
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9. A. G. Plant, V. Najdanović-Visak, M. J. Joyce, Bor Kos, Anže Jazbec, Luka Snoj, "In-situ acid generation to catalyse solketal production from glycerol using ionizing irradiation from a TRIGA reactor", In: *NENE 2020, 29th International Conference Nuclear Energy for New Europe, September 7-10, Portorož, Slovenia*, Proceedings, Nuclear Society of Slovenia, 2020, 1108.
10. Branislav Vrban *et al.* (16 authors), "Concept of education and training provided by the European nuclear experimental educational platform (ENEEP)", In: *NENE 2020, 29th International Conference Nuclear Energy for New Europe, September 7-10, Portorož, Slovenia*, Proceedings, Nuclear Society of Slovenia, 2020, 1607.

Theses and Mentoring

1. Anže Jazbec, *Calculation of gamma and neutron dose field inside the JSI TRIGA Mark II reactor hall:* doctoral dissertation, Ljubljana, 2020 (mentor Luka Snoj).

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 the computing, communication, data and security infrastructure for our research departments, centres and services at the Institute and participates in national and international collaborations.

Head:
Dr. Jan Jona Javoršek

The NIC's 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 the 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 ICT infrastructure, computing facilities and services. The NIC is responsible for four domains: networking infrastructure, network security, network services and distributed network supercomputing.

Networking Infrastructure. The Networking Infrastructure Centre is responsible for the development and management of the Institute's network backbone as well as departmental networks and physical infrastructure, providing access to internal services, external connections and the Internet. It manages the wireless networks and dedicated networks for the many services, projects and activities (i.e., dedicated links to other institutions, secure links to the Reactor Infrastructure Centre Podgorica, connections to scientific VPNs through GÉANT etc.).

Physical Network: In 2020 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. With the introduction of dedicated 100 Gbit/s double connections to Arnes' network we have increased the bandwidth available for dedicated connections for projects and for accessing major supercomputing and storage services. We implemented extensions and optimisations of the Institute backbone network as well as the expanded 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 external contractors. External connections have been optimised to support high network throughput work and experiments needed for collaboration 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.

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.

Monitoring: We adjusted and expanded our traffic, event and status-monitoring infrastructure, implemented on the basis of Nagios software packages for monitoring and alerting, Ganglia, Cacati and Observium for network monitoring, a customised dynamic analytical visualisation package build with Kibana and ElasticSearch, and Grafana-based aggregated monitoring with customized plug-ins to display an integrated report and react to usage fluctuations and unexpected events in the domain of web services, security policies, firewalls, authentication and authorization, network time systems, e-mail delivery, analysis, processing and security systems, physical machine sensory status, environmental data, power-line data, etc.

Wireless network: Thanks to modern, highly efficient components and central control modules we were able to continue to improve the wireless coverage and density of our wireless networks where usage is most condensed.

Figure 1: Traffic on the general network has been intense throughout the year, while the dedicated networks have seen expanded traffic due to new connectivity.

Network Security. The NIC manages security measures and policies at the external network border, in the internal network and regarding the services and software deployments for the users. External network security is implemented with the dynamic management and configuration of active firewall systems and routing configurations, while dedicated links are managed with passive measures (configuration, filtering and supervision) to facilitate high throughput. Constant dynamic supervision, traffic monitoring and event analysis is needed to ensure suitable security in the complex constraints and requirements of an open academic network that collide with current security considerations and demands for high throughput. 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.

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.

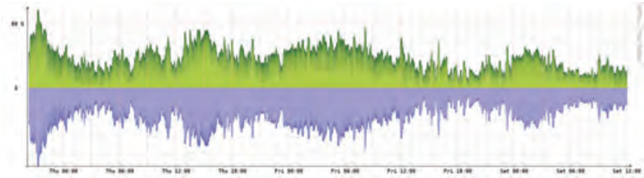

Figure 2: The new 100 Gbit/s connectivity shows high throughput at the JSI Computing Facility Teslova.

Figure 3: Additional computing cabinets and supporting infrastructure allowed for an upgrade of the NSC HPC cluster and the installation of the new Arnes HPC cluster, the most powerful public system in Slovenia at the time of installation.

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 with the in-house software development of Amavisd, the open-source e-mail content filter, and its SpamAssassin package integration, but also with continuous improvements in the support for new and advanced features in e-mail message and protocol stack handling and filtering.

Cryptography and certification: We have continued with the gradual integration of DNSSEC-signed internet domain names using automated mechanisms for the verification of the signatures and with the gradual introduction of the DANE system (integration of TLS certificates with the DNS system) in e-mail transfers and publishing SSHFP records via DNS servers. The number of 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 steadily 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 to support 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 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.

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. To meet the demands of growing data sets, these need to be complemented with an infrastructure supporting intensive high-performance computing and data analytics.

In 2020 we expanded the infrastructure for computationally intensive systems in the new computing centre at Teslova, established in 2015, with a new row of computing cabinets, but are still limited with the 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.

At the NIC computing centre at Jamova, where we can provide highly reliable cooling, network connectivity and uninterrupted power supply for critical services, we have added new cabinets and we continue to use the centre to host new servers from several departments. We have also expanded our web hosting activity (over 130 distinct sites).

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 super-computing. In the field of network-computing technology and infrastructure, high-throughput computing, high-performance computing, network and grid middleware, vectorisation, software containers, virtualisation and ICT as a service (cloud) continued to converge, which confirmed our strategy of integrating all of the above approaches. The NIC has continued to maintain central computing facilities for the JSI and has been collaborating with our other computing clusters while taking part directly in the Slovenian National Supercomputing Network SLING as a founding member and core partner, participating in development and integration efforts of the consortium as well as the participation in the EUROCC project. The NIC maintains the Slovenian certification agency SLING CA for science, research and grid computing, takes part in the maintenance and support of the core national supercomputing grid network services and coordinates work with international infrastructure projects and collaborations.

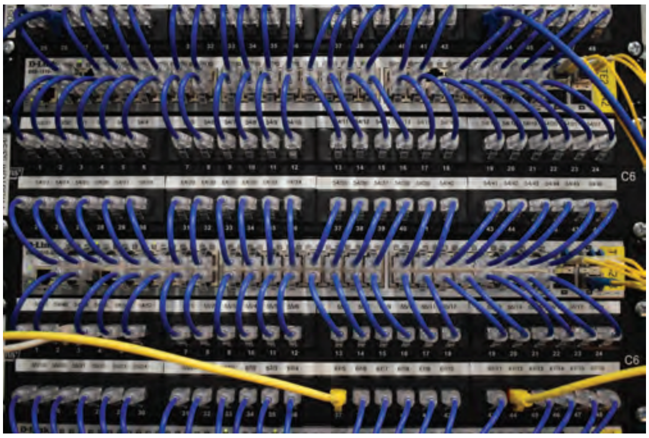

Figure 4: Modern cabling with custom patching cables allow us to deliver clean, easy to maintain network set-ups, as seen in this network cabinet at Teslova.

In 2020 the New System Cluster (NSC), the common computing cluster in the facilities of the Jožef Stefan Institute's Computing Centre Teslova, has continued to see a steady increase in user demand. The cluster with 1984 64-bit computing cores, 16 GPGPU accelerators (NVidia Kepler 40), almost 9 TB RAM and 90 TB disk storage has become too small and old to meet all the demand, so it has been upgraded with almost 2 PB of distributed CEPH-based storage and new computing nodes, provided in collaboration with the E7 department, bringing new AMD Epyc processors, NVidia Ampère 100 accelerators and Xilinx FPGA cards. Additionally, the centre now hosts the new Arnes HPC system, the largest publicly available HPC cluster in Slovenia at the time of the installation. In the context of this work, besides supporting users of JSI clusters, we also work on the integration of clusters with the national supercomputing network SLING using the NorduGrid ARC Grid Middleware to enable users to use all the resources in the network with the same interfaces and to use software containers to facilitate portability of the user software.

In the domain of network supercomputing we have been most involved with the Slovenian National Supercomputing Network (SLING), but we also worked within the European Grid Initiative EGI, PRACE (Partnership for Advanced Computing in Europe), EuroHPC initiative, notably the EuroHPC Vega and EuroHPC Leonardo hosting entity consortium, 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 of research projects and applications, among others in high-energy physics, medical sensor and image analysis, theoretical physics, astrophysics, biochemistry, protein-folding simulations, crystal analysis, knowledge technologies, artificial intelligence, statistical analysis and fluid dynamics, computational linguistics etc. In a number of cases we have been involved as part of the SLING support group in the parallelization and preparation of computing tasks and administration of the required run-time environments. Members of the NIC have also contributed as advisers in 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 successful Slovenian candidacy for a 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 - Educational, Audiovisual & Culture Executive Agency
2. H2020 - EUROCC; National Competence Centres in the Framework of EuroHPC
   Dr. Jan Jona Javoršek
   European Commission

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Technical officers

1. Jan Ivanjko, B. Sc.
2. **Dr. Jan Jona Javoršek, Head**
3. Barbara Krašovec, M. Sc.
4. Mark Martinec, B. Sc.

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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 biggest special libraries in Slovenia. We provide publication access, manage the Institute bibliography, and help our researchers to fulfil open-access-mandate requirements.

Head:
Dr. Luka Šušteršič

The peer-reviewed publication of results in scientific journals is an important, basic part of the research process. Therefore, access to literature is of vital importance for research quality and relevance. The information revolution and open-science movement 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 big publishers. We are a founding member of the ScienceDirect, SpringerLink, Wiley online library, IEEExplore 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 is stored in the COBISS database, which records the Institute's research since its founding in 1949. We manage 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 is 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.

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2. Marjan Verč, M. Sc.

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3. Suzi Korošec, B. Sc.
4. Jasna Malalan
5. Katarina Modic, B. Sc.
6. Alenka Ana Stante, B. Sc.
7. Jože Škulj
8. Branka Štrancar
9. Ana Tratnik
10. Saša Žnidar, B. Sc.

NEW CONTRACT

1. Consortium agreement for electronic journals procurement for 2020
   Dr. Luka Šušteršič
   Central Technical Library at the University of Ljubljana

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 in emissions of greenhousegases (GHGs). The centre is a focal point for the collection and transfer of energy-efficiency technologies to energy users, the state, energy service and equipment providers, and other interested agencies. At the same time, it covers the environmental effects of energy use and conversion. The most significant part of the EEC's activities is thus cooperation with state institutions in the preparation of strategic documents and legislation in the field of efficient energy use, energy planning, distributed electricity production and emission trading. Nevertheless, it still remains strongly connected, by its consulting and training role in energy, with industrial companies and other institutions as well as also being more and more involved in European research projects.

Head:
Stane Merše, M. Sc.

Energy and the Environment

In 2020 the EEC with its professional work ensured high-quality support to ministries in the preparation of the strategic development documents and the 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 energy efficiency for the period 2014–2020 for 2018 was prepared. The EEC was leading the consortium for the preparation of the analytical basis and draft of the National Energy and Climate Plan (NECP) of Slovenia, which was approved in February 2020 and continued preparation of the Long-term renovation strategy to support the renovation of national building stock into a highly energy efficient and decarbonised building stock by 2050.

Research and development work of the Energy Efficiency Centre is an important contribution to the preparation of key documents in Slovenia in the field of energy development, energy efficiency, renewables exploitation and the transition of Slovenia to a carbon-neutral society, with training activities and support to industry it significantly contributes to an increase of competitiveness and development restructuring.

Within the expert support of the Ministry of environment and spatial planning, EEC activities focused on the preparation of draft Long term climate strategy for Slovenia till 2050, based on the analytical basis and long-term GHG emissions' projection within the LIFE ClimatPath2050 project, with the goal to contribute to better climate governance through enhanced monitoring and planning of GHG mitigation measures in buildings, transport, industry, agriculture, forestry and waste. The third 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.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 the analytical basis for international reporting in the framework of the MMR, preparation of the Fourth biannual report for Slovenia (4BR) and continued preparation of the professional support for the design of National Air Pollution Control Programmes (NAPCP) prescribed by the NEC directive.

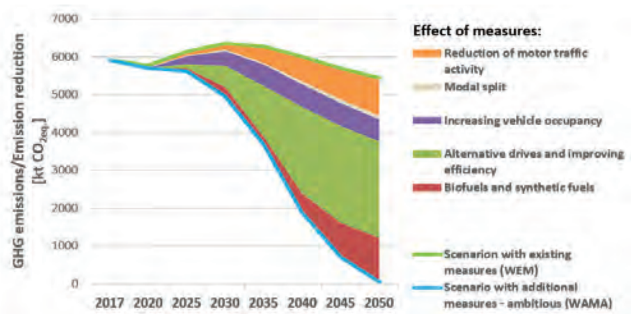

Figure 1: Assessment of different measures for a decrease of GHG emissions in transport (LIFE Climatepath2050).

The EEC cooperates with the Statistical Office of the Republic of Slovenia, where it annually prepares a model calculation of for fuels and energy use in households for the national energy statistics. 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 EEC set new reference electricity generation costs for the support scheme for RES and cogeneration electricity production units.

Promotion of Efficient Energy Use and Energy Consulting

In 2020 the EEC continued with its training activities, where already thirteenth cycle of energy managers training started within the European programme EUREM. Due to a very positive reaction of participants and their

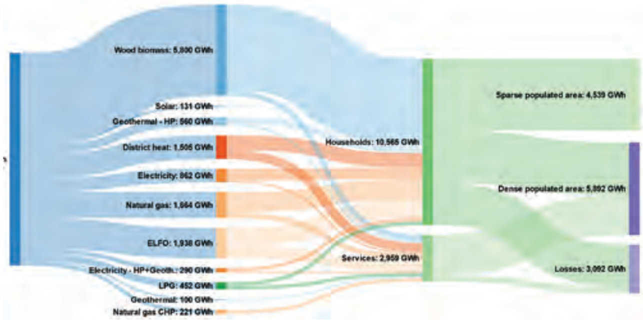

Figure 2: Building heating structure in Slovenia in 2017

Figure 3: Solar potential test field on the roof of SIJ-Acroni plant (project CREATORS).

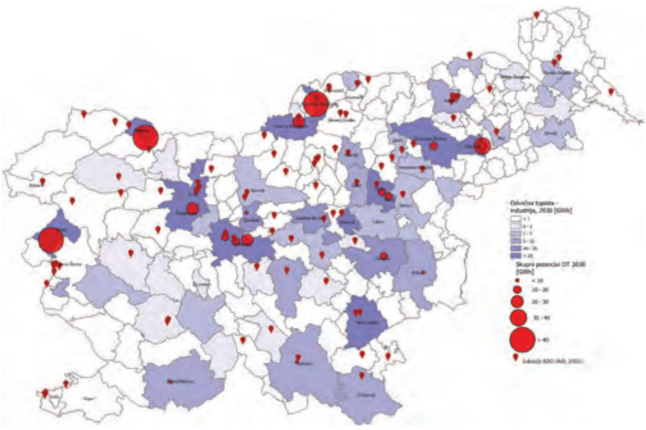

Figure 4: GIS presentation of industrial waste heat potentials for the reference year 2030 (heat map JSI-EEC)

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 2020 the EEC continued its intensive development work in the field of district heating (DH) and successfully finished a Benchmark Study of District Heating Companies, where a detailed analysis of the operation and development of 13 DH systems in Slovenia was made. An intensive development of the GIS tool for the spatial analysis of heat consumption in buildings ("heatmap") continued and the EEC used the tool in the preparation of the Comprehensive assessment of the potential for efficient heating and cooling in Slovenia and a National heating and cooling strategy (Figure 4).

The EEC first prepared an environmental assessment of the project financed by green bounds in 2019 for SID bank and started the implementation of the extended energy audit of URI Soča buildings. EEC continued preparation of the "Strategy for energy and material efficiency and sustainable development of DARS d. d. by 2030" and professional cooperation with the company Plinovodi and the energy steel company Metal Ravne in field of waste-heat utilisation.

The EEC prepared the programme for the 22nd conference "Energy Managers Days", the annual meeting of energy managers with more than 200 participants confirms the quality and the public profile of the EEC professional work.

International Cooperation

In 2020 the EEC carried out 14 international projects, financed from European Union resources in the framework of LIFE, HORIZON 2020 ERASMUS+ and EUKI programme. 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 waste-heat recovery in industry (ETEKINA),
- Driving investment in energy-efficiency services through quality assurance (QualitEE),
- Monitoring indicators for energy use and energy efficiency in the EU – (ODYSSEE MURE),
- Improving the Performance of District Heating Systems in Central and East Europe (KeepWarm)
- Making heating and cooling for European consumers efficient, economically resilient, clean and climate-friendly (REPLACE)
- Creating Community Energy Systems – (CREATORS),
- 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),
- Carrying out the EU directive on renewable energy sources (CA – RES3).

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), draft Long-term climate strategy for Slovenia till 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.
2. **Establishment of energy-managers training** in the framework of the European project EUREM and **professional support to industry and other institutions** by carrying out energy audits, feasibility studies and other consulting (Goodyear, TE-TOL, Luka Koper, Salonit Anhovo, Telekom Slovenije, Letrika–Mahle, BTC, KOTO, etc.).
3. In the framework of the European project **Transparense** the EEC led, very successfully, the preparation of the **European code of Conduct for energy contracting**. The Code identifies the basic values and principles, which are of key importance for the successful preparation and carrying out of projects with third-party financing. The Code was very successfully accepted at the European level and currently already has 171 signatories, among them also the European association of companies for energy services (eu.ESCO) and the European federation for intelligent services of energy efficiency (EFIEES), supported also by the European Commission. In Slovenia the code was already tested in practice in a project of integrated energy renovation of the municipal building of the municipality Brda.

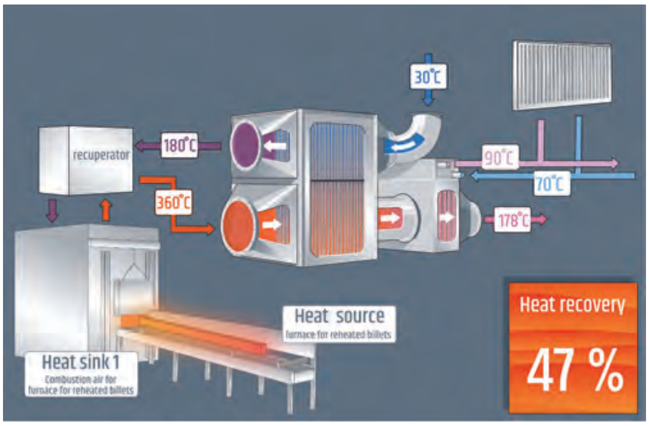

Figure 5: Waste-heat utilisation pilot unit scheme on the Allino furnace in company SIJ Metal Ravne, d.o.o (ETEKINA project).

Organization of conferences, congresses and meetings

1. Long-term climate strategy and local challenges, workshop on LIFE Climate Path 2050, RCP Brinje, February 12, 2020
2. EUREM educating, RCP, Brinje, March - May 2020 (due to COVID-19 only partially implemented in 2020, the rest in 2021)
3. Presentation of the draft Long-term Climate Strategy up to 2050 of Slovenia, Ljubljana, September 18, 2020 (co-organising with Ministry of the Environment and Spatial Planning)
4. Presentation of the background analysis for the Long-term Climate Strategy up to 2050 of Slovenia, LIFE Climate Path 2050, Ljubljana, September 24, 2020
5. Presentation of the draft Long-term Climate Strategy up to 2050 of Slovenia, Ljubljana, September 25, 2020 (co-organising with Ministry of the Environment and Spatial Planning)
6. 22nd Energy Days, Meeting of energy managers of Slovenia, 23. – 24. November 2021, virtual

Patent granted

1. Marko Matkovič, Iztok Tiselj, Ivo Kljenak, Andrej Prošek, Matjaž Leskovar, Ljubo Fabjan, Leon Cizelj, Method and apparatus for assessing the state of spent-fuel facility, GB2530969 (B), UK Patent Office, 08. 04. 2020.

INTERNATIONAL PROJECTS

1. Life IP Care4Climate - Boosting greenhouse gas emissions reduction by 2020 with a view to 2030
Stane Merše, M. Sc.
European Commission
2. European Climate Initative (EUKI) - EU Climate Action Dialogues
Katarina Trstenjak
Europäische Klimaschutzinitiative (euki)
3. ERASMUS+; EEE - Energy Efficiency Expert
Dr. Boris Sučić
Inapp - Istituto Nazionale Per L'analisi
4. „LIFE ClimatePath 2050" Slovenian Path towards the Mid-Century Climate Target
Andreja Urbančič, M. Sc.
European Commission
5. H2020 - QualitEE; Quality Certification Frameworks for Energy Efficiency Services to scale up Responsible Investment in the Building Sector
Damir Staničić, M. Sc.
European Commission
6. H2020 - KeepWarm; Improving the Performance of District Heating Systems in Central and East Europe
Stane Merše, M. Sc.
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

RESEARCH PROGRAMME

1. Modelling and environmental impact assessment of processes and energy technologies
Dr. Fouad Al-Mansour

R&D GRANTS AND CONTRACTS

1. Social acceptability of territorial effects in RES scenarios
Andreja Urbančič, M. Sc.
2. Investigation of turbulent heat transfer in an annulus through advanced experimental and computational methods
Asst. Prof. Marko Matkovič
3. Evaluation of greenhouse gasses mitigation measures in industry
Dr. Matevž Pušnik
4. Development and design of energy consuption monitoring by connecting various databases
Dr. Fouad Al-Mansour
5. Evaluation of greenhouse gasses mitigation measures in industry
Dr. Matevž Pušnik
Ministry of the Environment and Spatial Planning
6. Development and design of energy consuption monitoring by connecting various databases
Dr. Fouad Al-Mansour
Ministry of Infrastructure

NEW CONTRACTS

1. Analysis of eligibility and justification of creation of detailed plans with additional measures that can be funded through Just Transition Fund for Goriska, Gorenjska and Koroska Region with the aim to reach goals of the Just Transition
Dr. Boris Sučić
Golea, Nova Gorica
2. 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
3. Prepration of the 4th Biennial Report for the Conference of the Parties under UNFCCC
Matjaž Česen, B. Sc.
Ministry of the Environment and Spatial Planning
4. Energy Consumption of Slovenian Households Based on Model Calculation for 2019
Matjaž Česen, B. Sc.
Statistical Office of the Republic of Slovenia
5. Environmental impact assessment
Stane Merše, M. Sc.
Sid Banka, d. d., Ljubljana
6. Analysis and updating of data on planned natural gas consumption for the approval of the M6 Ajdovščina - Lucija pipeline project
Stane Merše, M. Sc.
Plinovodi d. o. o.

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1. Dr. Fouad Al-Mansour
2. Asst. Prof. Marko Matkovič
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5. Andreja Urbančič, M. Sc.

Postdoctoral associate
6. Dr. Matevž Pušnik

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19. Tadeja Janša, B. Sc.
20. Igor Ribič
21. Katarina Trstenjak, B. Sc.

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Original Article

1. Jurgita Malinauskaite, H. Jouhara, B. Egilegor, Fouad Al-Mansour, L. Ahmad, Matevž Pušnik, "Energy efficiency in the industrial sector in the EU, Slovenia, and Spain", *Energy*, 2020, **208**, 118398.
2. Marko Kovač, Matjaž Česen, Andreja Urbančič, Stane Merše, "Is there a chance to limit transport in Slovenia in the light of the climate change?: top down approach for personal vehicles", *International journal of environmental sciences and development*, 2020, **11**, 11, 499-503.

Published Conference Contribution

1. Andrej Trkov, Luka Snoj, Stane Merše, Johannes Teun van Elteren, Blaž Likozar, "A new paradigm on plastic waste (plastics - the problem or the solution)", In: *NENE 2020, 29th International Conference Nuclear Energy for New Europe, September 7-10, Portorož, Slovenia*, Proceedings, Nuclear Society of Slovenia, 2020, 601.
2. Boštjan Zajec, Anil Kumar Basavaraj, Blaž Mikuž, Boštjan Končar, Mohit Sharma, Marko Matkovič, "Experimental and numerical analysis of heat transfer on the annular test section", In: *NENE 2020, 29th International Conference Nuclear Energy for New Europe, September 7-10, Portorož, Slovenia*, Proceedings, Nuclear Society of Slovenia, 2020, 708.
3. Boštjan Zajec, Boštjan Končar, Marko Matkovič, Leon Cizelj, "Experimental investigation of subcooled flow boiling of R245fa in a narrow horizontal annular duct", In: *MHMT'20, 5th World Congress on Momentum, Heat and Mass Transfer, October 14 - 16, 2020*, Proceedings, International ASET Inc., 2020, 170.

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: Three decades of transitions in Central and Eastern Europe*, Elsevier, 2020, 247-282.

Professional Monograph

1. Barbara Petelin-Visočnik, Katarina Trstenjak, Andreja Urbančič, Polona Lah, Gašper Stegnar, Marko Kovač, Tadej Žaucer, Jože Verbič, *Podnebno ogledalo 2020: cilji v letu 2020 so prvi mejnik na poti v podnebno nevtralno družbo*, Institut "Jožef Stefan", 2020.

Patent

1. Marko Matkovič, Iztok Tiselj, Ivo Kljenak, Andrej Prošek, Matjaž Leskovar, Ljubo Fabjan, Leon Cizelj, *Method and apparatus for assessing the state of spent-fuel facility*, GB2530969 (B), UK Patent Office, 8. 04. 2020.

Theses and Mentoring

1. Gašper Stegnar, *Progressive building information modelling methodology for energy renovation of office buildings:* doctoral dissertation, Ljubljana, 2020 (mentor Tomo Cerovšek; co-mentor Marjana Šijanec Zavrl).

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 in the field of electron microscopy and microanalysis. Access to the research equipment of the CEMM is available to other JSI departments as well as other research institutions, universities and industrial partners. The equipment at the CEMM is used by researchers who are interested in the morphology and structural and chemical characterization of materials between the micrometre and the atomic levels.

Head:
Prof. Miran Čeh

Part of the centre was completely renovated and reorganized in 2020. The reason for the renovation was an optimization of the environment due to the purchase of two new scanning electron microscopes and to provide better working conditions for the microscopes' users and the centre's employees (Figures 1 and 2). At the CEMM there are three scanning electron microscopes (SEM) JSM-7600F, Verios G4 HP and Quanta 650, two transmission electron microscopes (TEM) 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 (transmission electron microscope with atomic resolution) at the National Institute of Chemistry.

In 2020 we began training operators on the new state-of-the-art Verios G4 HP high-resolution scanning electron microscope, Thermo Fisher Scientific (Figure 3). The microscope is the only one of its kind in this part of Europe and provides extremely high resolution at low excitation voltages. It also features automatic pattern insertion, the ability to observe non-conductive patterns, and exceptional Z-contrast even at low voltages. In addition to the highly sensitive EDXS detector, the microscope is equipped with a transmission detector (STEM) as well.

Figure 1: Centre for Electron Microscopy and Microanalysis (CEMM).

We also started training operators in 2020 on the new Quanta 650 electron microscope, Thermo Fisher Scientific (Figure 4). The main feature of this microscope is that it is operational 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 involving the equipment at the CEMM is diverse, with many different materials and the use of different analytical techniques.

- Scanning electron microscopy is employed to observe the morphology and structure of the surfaces and for the microstructural investigation and determination of the chemical composition. The most investigated samples are ceramics (polycrystalline oxide and non-oxide compositions), nanostructured materials, metallic magnetic materials, metals, alloys glass, etc. All of the scanning electron microscopes in the CEMM are equipped with an energy-dispersive (EDXS) and/or wavelength dispersive (WDXS) spectrometers for X-rays, allowing non-destructive determination of the chemical composition of the investigated materials. The scanning electron microscope JSM-7600F is additionally equipped with an electron back-scattered diffraction (EBSD) detector and an electron lithography system. The Verios 4G HP microscope enables the observation of the morphology of nanoparticles and samples extremely sensitive to electron doses and the observation of transmission samples (STEM). The Quanta 650 microscope allows the observation of larger, conductive or non-conductive samples.
- Transmission electron microscopy (TEM) provides an insight into the structure of the material on the nano-scale (atomic level). Transmission electron microscopy enables structural and chemical analyses of the grain boundaries and study of

Figure 2: Renovated room for the JSM-7600F microscope.

Figure 4: ESEM Quanta 650 microscope.

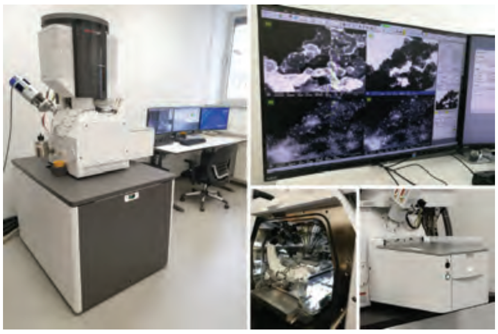

Figure 3: Verios 4G HP microscope.

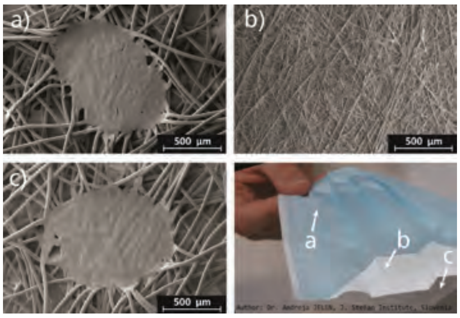

Figure 5: SEM image of polypropylene membrane (Jelen A., F5, JSM-7600F)

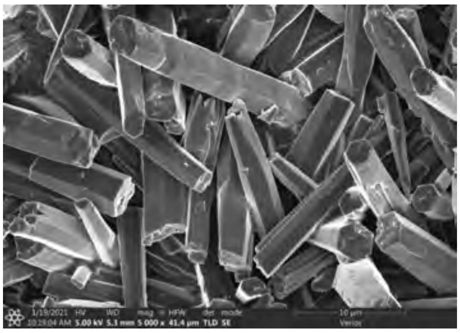

Figure 6: SEM image of $CaCO_3$ aragonite crystals (Samardzija Z., K7, Verios 4G HP).

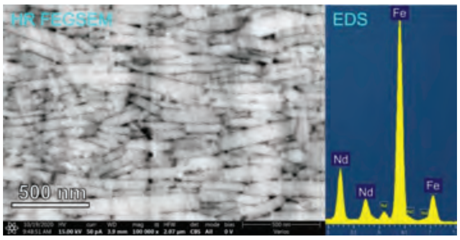

Figure 7: High-resolution BSE image and EDS analysis of NdFeB magnet (Samardzija Z., K7, Verios 4G HP).

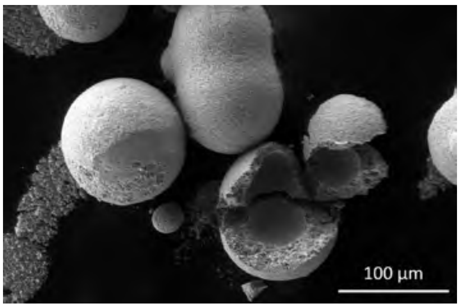

Figure 8: SEM image of granulate under low-vacuum conditions (Bernik S., K7, Koblar M, CEMM, Quanta 650).

precipitates, planar defects and dislocations. In addition to ceramic samples other materials and structures are investigated, such as thin films on different substrates, alloys, delicate metallic magnetic materials, polymers, etc. Transmission electron microscope JEM-2100 is equipped with an EDXS spectrometer and a CCD camera, and the JEM-2010F is additionally equipped with a scanning transmission electron (STEM) unit, EDXS and EELS (electron energy loss) spectrometers, and a CCD camera.

– The CEMM also manages the necessary equipment for SEM and TEM sample preparation.

The operation of the Centre is managed by properly trained employees. Besides maintenance of the equipment, other CEMM activities include, among others, the 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. CEMM personnel are also 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 using the CEMM equipment

The examples of analyses of structural and chemical characterisations of different materials using electron microscopy techniques were performed by the CEMM employees as well as operators from different JSI departments.

1. Polypropylene membrane analysis

A study of sterilization of polypropylene membranes in previously ionized face masks was performed. (Figure 5).

In: Pirker. L.; Pogačnik Kranjc. A.; Malec. J.; Radulović. V.; Gradišek. A.; Jelen. A.; Remškar. M.; Mekjavić. I.B.; Kovač. J.; Miran. M.; Snoj. L. Sterilization of polypropylene membranes of facepiece respirators by ionizing radiation. Journal of membrane science, 2021, 619, 118756

2. $CaCO_3$ aragonite analysis

SEM analysis of samples from water dispenser showed the presence of $CaCO_3$ aragonite crystals (Figure 6).

3. NdFeB magnet

NdFeB magnet analysis showed preferential grain orientation. The grains are below 1 micrometre in size (Figure 7).

4. Granulate

Internal structure of ZnO-based granules. The image was taken without spattering of the sample (Figure 8).

5. Microplastic fibres

Images of polymer fibres in the study of microplastic degradation (Figure 9).

6. WO_3 nanowires with IrO_2 particles

An SEM and TEM study of WO_3 nanoparticles coated with IrO_2 nanoparticles was performed, according to different synthetic procedures and according to different concentrations of crystalline IrO_2 nanoparticles on WO_3 nanoparticles (Figure 10).

In: Navarrete. E.; Bittencourt. C.; Umek. P.; Cossement. D.; Guell. F.; Llobet. E. Tungsten trioxide nanowires decorated with iridium oxide nanoparticles as gas sensing material. Journal of alloys and compounds, 2020, 812, 152156-1-152156-9

7. A study of the effect of TiO_2 nanoparticle properties on pneumonia

As part of the investigation of the influence of the physical and chemical properties of nanoparticles on pneumonia, TEM analyses of TiO_2 nanoparticles and nanotubes, nanocuboids and quartz were performed (Figure 11).

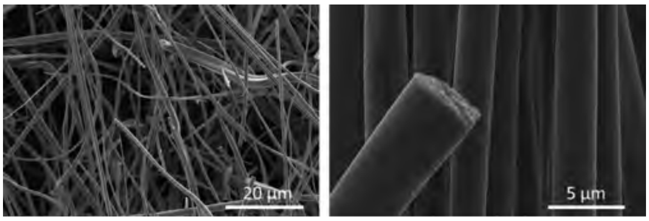

Figure 9: SEM image of fibres (Radošević T., K9, Koblar M, CEMM, Quanta 650).

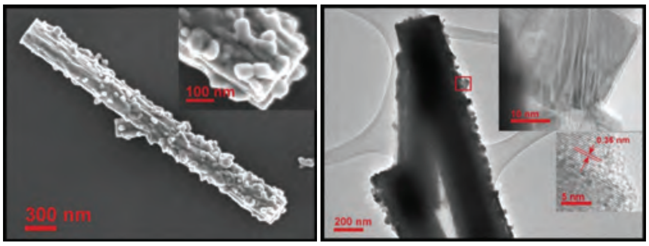

Figure 10: SEM and TEM image of WO_3 nanowires with IrO_2 nanoparticles (Umek P., F5, JEM-2100).

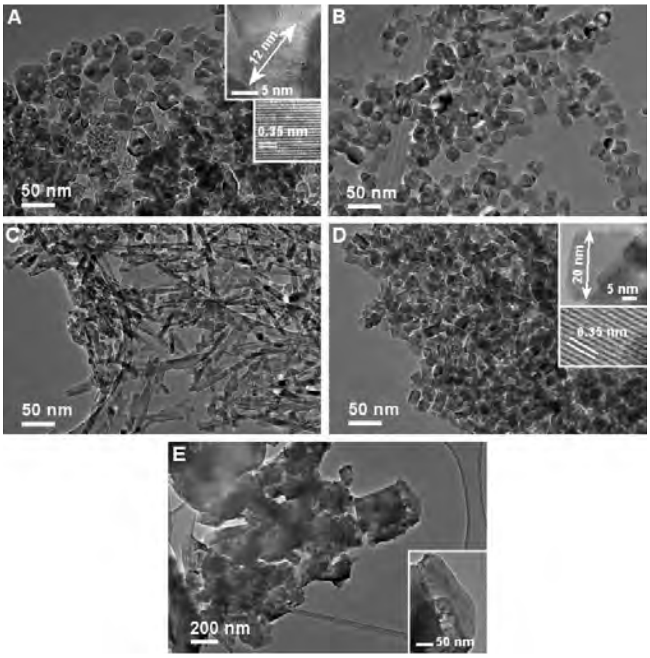

Figure 11: TEM images of commercial TiO_2 samples (A, B) on the laboratory scale of synthesized TiO2 nanotubes and nanocuboides (C, D) and commercial quartz sample DQ12 (Umek P., F5, JEM-2100).

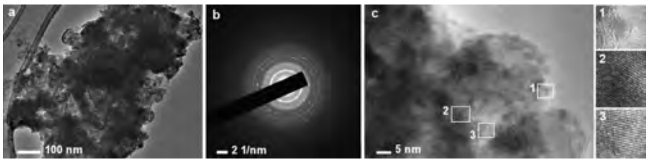

Figure 12: TEM study of layered Zn-Al hydroxide with Mo-doped TiO_2 nanoparticles (Umek P., F5, JEM-2100).

In: Danielsen. P.; Štrancar. J.; Umek. P.; Koklič. T.; Garvas. M.; et al. Effects of physicochemical properties of TiO_2 nanomaterials for pulmonary inflammation, acute phase response and alveolar proteinosis in intratracheally exposed mice. Toxicology and applied pharmacology, 2020, 386, 114830-1-114830-18

8. TEM study of Zn-Al hydroxide

TEM study of the morphological characteristics of layered Zn-Al hydroxide with Mo-doped TiO_2 nanoparticles in the interlayer space used in catalytic processes (Figure 12).

In: Cerc Korošec. R.; Miljević. B.; Umek. P.; Bergh. J. M. van der.; Vučetić. S.; Ranogajec. J. Photocatalytic self-cleaning properties of Mo:TiO_2 loaded Zn-Al layered double hydroxide synthesised at optimised pH value for the application on mineral substrates. Ceramics international, 2020, 46, 6756-6766

9. TEM study of TiON nanotubes

In TEM, a study of TiON nanotubes inside which Ir grains were trapped was performed. TiON analysis helped to complete a study of the effect of metallic Ir within TiON nanotubes on increasing the efficiency of catalytic reactions (Figure 13).

In: Bele. M.; Jovanovič. P.; Marinko. Ž.; Drev. S.; Šelih. V. S.; Kovač. J.; Gaberščček. M.; Koderman Podboršek. G.; Dražić. G.; Hodnik. N.; Kokalj. A.; Suhadolnik. L. Increasing the oxygen-evolution reaction performance of nanotubular titanium oxynitride-supported Ir nanoparticles by a strong metal-support interaction. ACS Catalysis, 2020, 10, 13688-13700

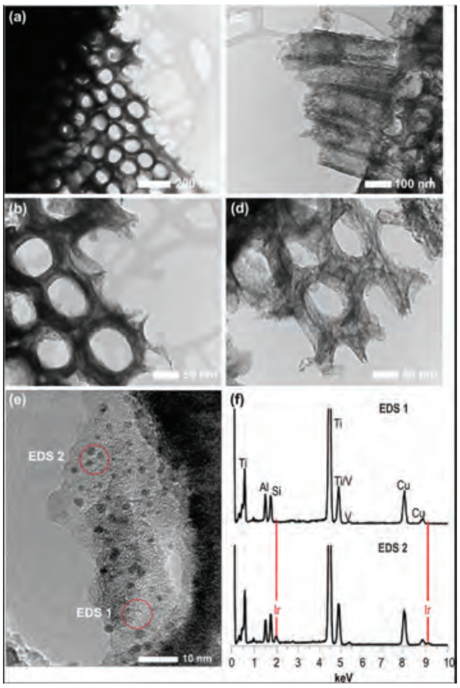

Figure 13: TEM images of TiON nanotubes: (a, b, d) top view and (c) side view of nanotubes. (e) TEM image of TiON nanotubes with Ir nanoparticles (f) and accompanying EDS analysis (Drev S., CEMM, JEM-2010F).

10. Adsorption of zinc on the surface of a carbon nanotube

TEM study of the position of zinc atoms and clusters of atoms absorbed on the surface of a carbon nanotube. HAADF and BF STEM analysis were performed (Figure 14).

11. Defects in $BiFeO_3$ domain walls

High-angle annular dark-field (HAADF) STEM images of DWs (a,c) with corresponding normalized distribution maps of Bi-column intensities before (b) and after the application of the electric field (d), respectively. These regions correspond to the areas marked with full orange boxes in panels (a,c). Insets in panels (a,c) show the Fe displacement directions (relative to the Bi sublattice) in the two adjacent domains, with dashed-yellow boxes indicating the DW regions.

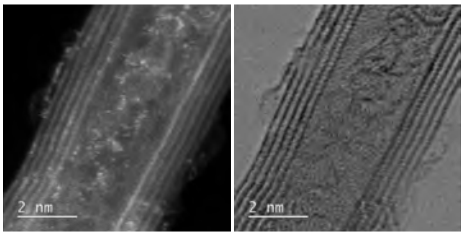

Figure 14: HAADF and BF STEM images of zinc atoms and clusters of atoms on the carbon nanotube (Makovec D., K8, JEM-ARM200F).

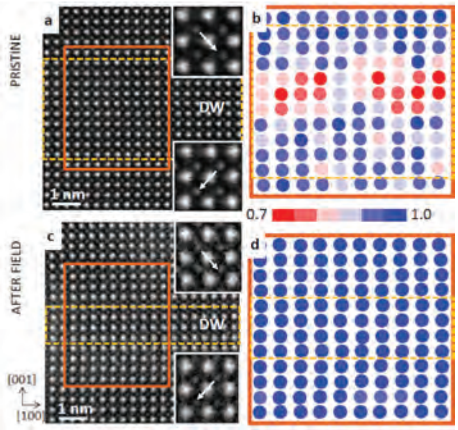

Figure 15: HAADF STEM images of domain wall in $BiFeO_3$ (Bencan A., Dražić G., K5, KI, JEM-ARM200F).

The reduction of the Bi-atom column intensities within the DW in pristine sample (b) indicates the presence of Bi vacancies. In contrast, no evidence of Bi-vacancy accumulation at the newly formed DW (d) was found after application of an electric field (Figure 15).

In: Benčan. A.; Dražić. G.; Uršič Nemevšek. H.; Komelj. M.; Rojac. T. Domain-wall pinning and defect ordering in $BiFeO_3$ probed on the atomic and nanoscale. Nature communication, 2020, 11, 1762-1-1762-8

12. High-precision determination of ZnO interface using DFT and HRTEM

High-precision determination of interface structures using ***ab-initio*** calculations (DFT) and high-resolution transmission electron microscopy (HRTEM). Two inversion-boundary (IB) structures in Sb_2O_3-doped ZnO: (**a**) the reported one (Rečnik ***et al***. 2001), based on single stacking fault, and (**b**) the new, more stable one, as predicted by DFT screening, that is based on a double-stacking-fault sublattice (Ribić ***et al.*** 2020). Combination of experimental and computational approaches allows a determination of fine structural details with confidence levels down to <1 pm. The study is a result of collaboration between the Institute for Multidisciplinary Research in Belgrade and Jožef Stefan Institute in Ljubljana. Experimental work was conducted at the CEMM in Ljubljana (Figure 16).

In: Ribić. V.; Rečnik. A.; Komelj. M.; Kokalj. A.; Branković. Z.; Zlatović. M.; Branković. G.; New inversion boundary structure in Sb-doped ZnO predicted by DFT calculations and confirmed by experimental HRTEM. Acta Materialia, 2020, 199, 633-648

13. High-precision determination of ZnO interface using DFT and HRTEM

A study of the growth and possible effects of voltage on ferroelectric domains in epitaxial heterostructures was performed (Figure 17 and 18).

In: Belhadi, J.; Gabor, U.; Uršič, H.; Daneu, N.; Kim, J.; Tian, Z.; Koster, G.; Martin, LW.; Spreitzer, M. Growth mode and strain effect on relaxor ferroelectric domain in epitaxial 0.67Pb(Mg1/3Nd2/3)O3-0.33PbTiO3/SrRuO3 heterostructures. RSC Adv., 2021, 11, 1222-1232

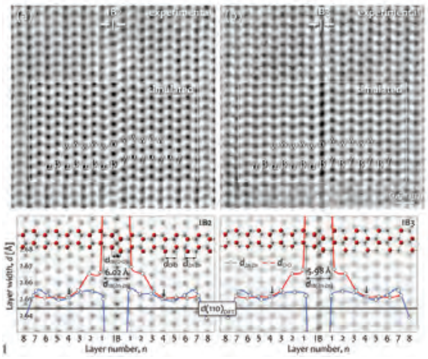

Figure 16: Two inversion-boundary (IB) structures in Sb_2O_3-doped ZnO: (a) the reported one (Rečnik et al. 2001), based on single stacking fault, and (b) the new, more stable one, as predicted by DFT screening, that is based on a double stacking fault sublattice (Ribić et al. 2020). (Rečnik A., Ribić V., K7, JEM-2010F).

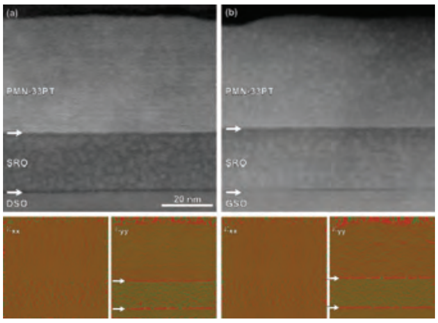

Figure 17: HAADF-STEM cross-section images of $0.67Pb(Mg_{1/3}Nb_{2/3})O_3/SrRuO_3/DyScO_3$ (a) and $0.67Pb(Mg_{1/3}Nb_{2/3})O_3/SrRuO_3/GdScO_3$ (b) heterostructures and their corresponding GPA analysis of the in-plane (ε_{xx}) and out-of-plane (ε_{yy}) lattice strains (Daneu N, K9, JEM-ARM200F).

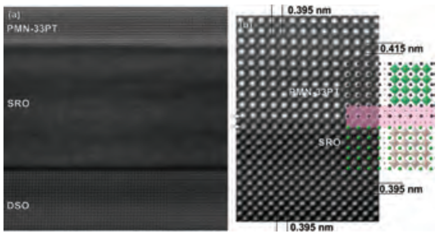

Figure 18: (a) Filtered HAADF-STEM image of the $0.67Pb(Mg_{1/3}Nb_{2/3})O_3/SrRuO_3/DyScO_3$ heterostructure showing a continuous transition of atomic columns from the substrate across the two interfaces without the presence of dislocations. The DSO–SRO contact is sharp and follows single atomic layer, whereas the SRO/PMN-33PT heterointerface makes steps to neighbouring atomic planes (atomic mixing at the A-sites and B-sites is likely). (b) Local atomic structure of the SRO/PMN–33PT heterointerface, where the SRO layer ends with the B-site layer (RuO_2) and the PMN–33PT layer starts with the A-site layer (PbO). Tilting of RuO_6 and perhaps also the $((Mg_{2/9}Nb_{4/9}Ti_{3/9})O_6)$ octahedra directly at the contact is likely (pink region) (Daneu N, K9, JEM-ARM200F).

INTERNATIONAL PROJECTS

1. H2020 - EUROfusion; Education-ED-FU
   Prof. Miran Čeh
   European Commission
2. Investigation of Helium Retention in Plasma Facing Materials Using Advanced Analytical Methods
   Andreja Šestan Zavašnik, B. Sc.
   Slovenian Research Agency

R&D GRANTS AND CONTRACTS

1. Nanoscale investigations of diffusion controlled topotaxial phase transformations in rutile-corundum host systems
   Dr. Sandra Drev

NEW CONTRACT

1. BIO1-2020
   Prof. Miran Čeh
   Lek d. d.

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3. Dr. Jitka Hreščak

Postgraduate
4. Andreja Šestan Zavašnik, B. Sc.

Technical officer
5. Maja Koblar, B. Sc.

BIBLIOGRAPHY

Original Article

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2. Blaž Leskovar, Zoran Samardžija, Maja Koblar, Iztok Naglič, Boštjan Markoli, "Development of an Al-Mn-Si-based alloy with an improved quasicrystalline-forming ability", *JOM: The journal of minerals, metals and materials society*, 2020, **72**, 4, 1533-1539.
3. Sabina Markelj, Thomas Schwarz-Selinger, Matic Pečovnik, W. Chromiński, Andreja Šestan, Janez Zavašnik, "Deuterium transport and retention in the bulk of tungsten containing helium: the effect of helium concentration and microstructure", *Nuclear fusion*, 2020, **60**, 10, 106029.

CENTRE FOR KNOWLEDGE TRANSFER IN INFORMATION TECHNOLOGIES CT-3

The Centre for Knowledge Transfer in Information Technologies performs educational, promotional and infrastructural activities and provides for the direct exchange of information and experience between researchers and the users of their research results. The centre has thirteen researchers and technical staff working in the areas of research-results dissemination and eLearning. In particular, the centre is well known by the 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 the analysis and visualization of large bibliographic and project databases. The centre is covering the management, training and dissemination activities of several EU projects.

Head:
Mitja Jermol, M. Sc.

In 2020 we were active in the following projects from the H2020 programme: WATER4CITIES (Holistic Surface Water and Groundwater Management for Sustainable Cities), MEET CINCH (A Modular European Education and Training Concept In Nuclear and RadioCHemistry), X5GONE (Cross Modal, Cross Cultural, Cross Lingual, Cross Domain, and Cross Site Global OER Network), THEYBUYFORYOU (Enabling procurement data value chains for economic development, demand management, competitive markets and vendor intelligence) DATABENCH (Evidence Based Big Data Benchmarking to Improve Business Performance), PerceptiveSentinel (BIG DATA Knowledge Extraction and re-creation Platform), ELEXIS (European Lexicographic Infrastructure), SILKNOW (Silk heritage in the Knowledge Society: from punched cards to big data, deep learning and visual/zangible simulations), COG-LO (COGnitive Logistics Operations trough secure, dynamic and ad-hoc collaborative networks), EnviroLENS (Copernicus for Law Enforcement Support), FIN-TECH (A FINancial supervision and TECHnology compliance training programme), 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), Humane AI (Toward AI Systems That Argument and Empower Humans by Understanding US our Society and the World Around), INFINITECH (Tailored IoT & BigData Sandboxes and Testbeds for Smart, Autonomous and Personalized Services in the Europe), FACTLOG (Energy-aware Factory Analytics for Precess Industries), A-CINCH; Augmented Cooperation in Education and Training in Nuclear and Radiochemistry) in ERASMUS+: Micro HE (Support Future Learning Excellence through Micro-Credentialing in Higher Education) in MentorTrain (Training and Equipping Mentors in SMEs to provide Quality Apprenticeships).

In 2020 we participated in nineteen European projects.

The centre prepares and organizes educational events, such as conferences, seminars, workshops, and summer schools. They are targeted at experts who would like to apply the latest knowledge and achievements from intelligent data analysis, knowledge technologies, data mining, text mining and decision support to the areas of network organizations, business decisions, finance, marketing. A special consideration is put on managers and decision makers who are aware of the strengths and benefits to the success of their business. All educational events are designed to transfer the basic, additional and latest expert knowledge to the companies, research and educational organizations.

To make the knowledge transfer efficient we are combining traditional and ICT-supported training methods. For this purpose we are operating a number of training web portals. The most popular one is http://videolectures.net/. It now offers 27,681 recorded tutorials from different scientific events. The main purpose of the portal is to provide free and open access to high-quality video lectures presented by distinguished scholars and scientists at the most important and prominent events. In today's world VideoLectures.NET represents a free knowledge hub, a way of opening up education to everyone for everyone and as there is a great need to share educational content on all levels to benefit society and foster the economy. It also gives a learning opportunity to audiences from all social levels.

Figure 1: Open Education for a Better World (OE4BW)

VideoLectures.Net has strong connections in Open Cast Foundation, Open Course Ware Consortium and Knowledge 4 All Foundation Ltd.

In 2020, 883 new individual lectures were published on Videolectures.Net. Due to the Covid 19 pandemic restrictions, most lectures scheduled for 2020 were cancelled. As a result, the Videolectures.Net changed its approach to include support for organizing online conferences, live streaming of lectures, and technical facilitation of so-called hybrid events.

The biggest conferences we have published in 2020 are:

– ESWC 2020 Conference
– ACML2020 Conference
– PAKDD2020 Conference

In addition, we continued to collaborate on content-creation projects such as A- CINCH and maintained long-term partnerships, even though the dates of some events shifted. Videolectures also continued to collaborate in publishing seminars from the JSI, the Faculty of Architecture, the Positive Psychology series and content recorded at the Ministry of Education, Science and Sport, to name just a few.

In addition to publishing new content to the repository, we completed or enabled the execution of all Videolectures.Net related tasks in projects: MeetCINCH, Mentortrain, and X5GON.

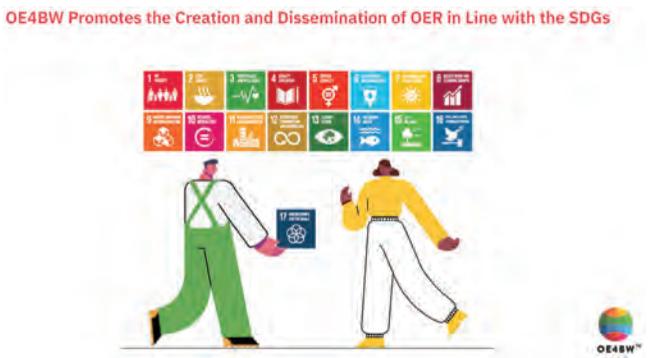

Figure 2: OE4BW addresses UN SDGs

Videolectures.Net also developed a mobile application, which is already publicly available and in the testing phase.

We provided dissemination channels for the Water4Cities project, including secondments to the coordinator's institution.

Spring 2020, along with the pandemic COVID -19, also brought us for the first time the virtual organization and execution of the 15th ACM Competition in Computer Science and Information Technology. All the participants were simultaneously given access to the competition systems of ACM Slovenia (https://rtk.fri.uni-lj.si/ and https://putka-rtk.acm.si/), while they were present throughout the competition, for any questions are also available Organizing Committee and computers and Informatics Competition Commission. A total of 168 students from 24 secondary schools and three independent institutions participated in the area of computer science (programming), 16 students competed in the area of web-application development, and 5 participants took the challenge in the offline task. We also receive a few educational videos each year, this time from four elementary schools, thirteen high schools, and eleven colleges. The results of the competition can be found at http://rtk.ijs.si/2020/rezultati.html, and each year we also award prizes for the best practical work. In the school programming competition we held in January, 306 students from all over Slovenia took part.

In 2020, as part of the international mentoring program for open education called "Open Education for a better world - OE4BW", we completed the third cycle with 82 projects developed and received the Award for Excellence for our efforts from the Open Education Global Community.

In 2020 we continued with the Water4Cities (Integrated Surface and Groundwater Management for Sustainable Urban Development) project under the European Horizon 2020 Marie Skłodowska Curie RISE project together with Laboratory for Artificial Intelligence (E3). We analysed data on groundwater, rivers and stormwater flow data in the Ljubljana aquafier and water quality and consumption on the Greek island of Skiathos. We continued with the development of models and a platform that will allow us to monitor optimal water management in real time. In 2020 we recorded and published regular webinars and interviews with our consortium partners as well as all the public presentations of the project, which are available on the Videolectures.NET subpage - http://videolectures.net/water4cities/.

A part of CT3, the UNESCO Chair on Open Technologies for Open Educational Resources and Open Learning, has in collaboration with the University of Nova Gorica, developed the international online mentoring program Open Education for a Better World. The programme promotes the creation and dissemination of Open Educational Resources (OER) in line with the UN Sustainable Development Goals (SDGs)

Since its beginnings in October 2017, the OE4BW mentoring programme has gained a steadily growing network of OER practitioners and experts from all over the world.

Due to the increased number of participants from around the world, we organized five regional Hubs – North America, South America, Europe, Africa and Asia – and one thematic Hub titled SDG 7 Hub that focuses on access to affordable, reliable, sustainable and modern energy sources.

We ended 2020 with 82 developed projects and were awarded for our efforts with the Open Collaboration Award from the Open Education Global Community. In July, we organized an online event called "OE4BW Eduscope 2020", which took place entirely online at the MiTeam platform and was attended by 470 participants from 26 countries.

Find out more about the programme, the projects and the developers at **https://oe4bw.org/**.

The CyberSANE project (Cyber Security Incident Handling, Warning and Response System for the European Critical Infrastructures) started in 2019, and the project 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.

In 2020 we started working with partners to develop technology to capture and analyze structured and unstructured data from the so-called dark web and from media articles. 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.

In 2020 we completed our role in the implementation of video content within the online repository Videolectures.net in the Erasmus + project "Training and equipping mentors in small and medium-sized enterprises to ensure quality apprenticeships" (Mentortrain). In 2020 we and our partners completed the post-production of a module for educating vocational school mentor mentors across Europe.

In the scope of the project "A Modular European Education and Training Concept In Nuclear and RadioCHemistry Courses" (Meet-Cinch) in 2020, Videolectures.Net recorded and published 45 courses. Our centre is collaborating with the Department of Environmental Sciences at the JSI in the development and design of extensive courses in the field of radiochemistry. The project has since concluded, but it will be continued through the activities of the newly approved project A-Chinch, in which the role of Videolectures is in producing video content.

This year, the International Research Center on Artificial Intelligence (IRCAI), led by representatives of our CT3 Center and the E3 Section, was launched at the JSI.

Work on project "Support Future Learning Excellence through Micro-Credentialling in Higher Education" (MicroHE) focused in 2020 mostly on finishing the tasks of the technical work package, which we are leading. In 2020 we achieved all the objectives of the work package we are leading and have improved and tested the developed solution (the micro-credentials metadata standard and a micro-credentials clearinghouse).

The EU H2020 project COG-LO (COGnitive Logistics Operations through secure, dynamic and ad-hoc collaborative networks) is aiming to create the framework and tools that will add cognition and collaboration features to future logistics processes. 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 Cognitive Logistics Object (CLO) based on the reference implementation model. We were also involved in the project pilots, especially in the pilot of the Post of Slovenia and the Croatian Post. The idea is that the project gets data streams that will help in defining the necessary cognitive methods and optimization algorithms. Due to the covid 19 pandemic the final system installation testing and execution of the test scenarios was interrupted, but will continue in 2021. Since the pandemic caused an increase in the delivery of shipments by 100% or more, an additional scenario for the Slovenian pilot was defined, this is processing same-day delivery requests and the management of increased short-term delivery demand based on cognitive logistics. Within the dissemination and exploitation activities, we presented the project and the Cognitive Adviser tool at the virtual conference Parcel+Post Expo 2020.

The EU H2020 project INFINITECH (Tailored IoT & BigData Sandboxes and Testbeds for Smart, Autonomous and Personalized Services in the European Finance and Insurance Services Ecosystem) aims at lowering 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 were involved in the pilot that will develop a platform for improving the effectiveness of the existing supervisory activities in the area of anti money laundering and combating terrorist financing (AML/ CTF) by processing a large quantity of data (Big Data) owned by the Bank of Slovenia (BS) and other competent authorities. In the future INFINITECH will establish a market platform that will provide access to the project's solutions, along with a Virtualized Digital Innovation Hub (VDIH) that will support innovators (FinTech/InsuranceTech) in their BigData/AI/IoT endeavours.

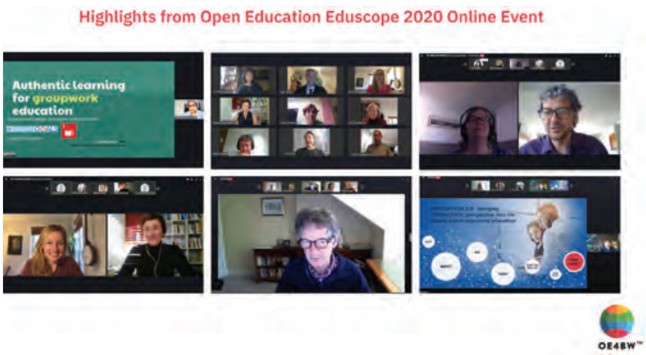

Figure 3: OE4BW Eduscope 2020

In 2020 we completed the European Horizon 2020 project TheyBuyForYou (Enabling procurement data value chains for economic development, demand management, competitive markets and vendor intelligence). As part of the project we worked with our partners to develop a data warehouse (Knowledge Graph) that contains data on public procurement in many European countries. The data warehouse is freely accessible and compatible with the OCDS standard (Open Contracting Standard). As part of the project, the JSI developed an online platform to analyse public procurement and public money spending. In the process we collaborated with the Ministry Public Administration, which aims to ensure transparency in the use of public funds and prevent corruption and other irregularities in the use of public funds. Our platform enables the detection and visualization of anomalies in public procurement and financial transactions and is available at http://tbfy.ijs.si.

In 2020 we are setting up a website with information about the coronavirus, and we are also setting up an infrastructure for free videoconferencing (all you need is a web browser): https://ustavimokorono.si/videokonferencni-sistem-jitsi/

We have also prepared a document with instructions and links for posting videos on the videolectures.net portal, where we are hosting videos created by teachers and others for the purpose of continuing educational and other processes during the actions to contain the spread of the Covid 19 virus. http://videolectures.net/site/news/COVID -19_online/

Awards and Appointments

1. In 2020, as part of the international mentoring program for open education called "Open Education for a better world - OE4BW", we completed the third cycle with 82 projects developed and received the Award for Excellence for our efforts from the Open Education Global Community.

Organization of conferences, congresses and meetings

1. Technical meeting of the EU project H2020 Silknow, Ljubljana, 10. 2. 2020
2. 15th Student competition in computer science, Ljubljana, Ljubljana, 27. 3. 2020 (virtual)
3. Organization of workshop "OE4BW 2020", 29. 6. - 3. 7. 2020 (virtual)
4. Organization of event "Dinamic coalition", 2020, 23. – 24. 7. 2020 (virtual)
5. Organization of the event OE4BW Eduscope 2020, 13. – 14. 10. 2020 (virtual)

INTERNATIONAL PROJECTS

1. ERASMUS+: Micro HE - Support Future Learning Excellence through Micro-Credentialing in Higher Education
   Mihajela Črnko
   European Commission
2. INEA/CEF - MARCELL, Multilingual Resources for CEF.AT in the Legal Domain
   Mitja Jermol, M. Sc.
   Innovation And Networks Executive Agency (inea)
3. ERASMUS+; MentorTrain - Training and Equipping Mentors in SMEs to provide Quality Apprenticeships
   Mihajela Črnko
   European Commission
4. H2020 - Water4Cities; Holistic Surface Water and Groundwater Management for Sustainable Cities
   Mitja Jermol, M. Sc.
   European Commission
5. H2020 - MEET-CINCH; A Modular European Education and Training Concept in Nuclear and RadioChemistry
   Mihajela Črnko
   European Commission
6. H2020 - X5gon; Cross Modal, Cross Cultural, Cross Lingual, Cross Domain, and Cross Site Global OER Network
   Mitja Jermol, M. Sc.
   European Commission
7. H2020 - PerceptiveSentinel; BIG DATA Knowledge Extraction and Re-creation Platform
   Mitja Jermol, M. Sc.
   European Commission
8. H2020 - DataBench; Evidence Based Big Data Benchmarking to Improve Business Performance
   Mitja Jermol, M. Sc.
   European Commission
9. H2020 - TheyBuyForYou; Enabling Procurement Data Value Chains for Economic Development, Demand Management, Competitive Markets and Vendor Intelligence
   Dr. Matej Kovačič
   European Commission
10. 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
11. H2020 - COG-LO; COGnitive Logistics Operations through secure dynamic and ad-hoc collaborative networks
    Mitja Jermol, M. Sc.
    European Commission
12. H2020 - EnviroLENS; Coprenicus for Environmental Law Enforcement Support
    Mitja Jermol, M. Sc.
    European Commission
13. H2020 - Humane AI; Toward AI Systems That Augment and Empower Humas by Understanding Us, our Society and the World Around Us
    Mitja Jermol, M. Sc.
    European Commission
14. H2020 - FIN-TECH; A FINancial supervision and TECHnology compliance training programme
    Mitja Jermol, M. Sc.
    European Commission
15. H2020 - NAIADES; A Holistic Water Ecosystem for Digitisation of Urban Water Sector
    Mitja Jermol, M. Sc.
    European Commission
16. H2020 - CyberSANE; Cyber Security Incident Handling, Warning and Response System for the European Critical Infrastructures
    Mitja Jermol, M. Sc.
    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
    Mitja Jermol, M. Sc.
    European Commission
18. H2020 - FACTLOG; Energy-aware Factory Analytics for Precess Industries
    Mitja Jermol, M. Sc.
    European Commission
19. H2020 - A-CINCH; Augmented Cooperation in Education and Training in Nuclear and Radiochemistry
    Mihajela Črnko
    European Commission
20. H2020 - ELEXIS; European Lexicographic Infrastructure
    Mitja Jermol, M. Sc.
    European Commission

R&D GRANTS AND CONTRACTS

1. Videorecording and Post-Processing
   Mitja Jermol, M. Sc.
2. CLARIN - European Research Infrastructure for Language Resources and Technology
   Mitja Jermol, M. Sc.
   Clarin Eric
3. Recording, Publishing and Disseminating of the Scientific Content of the EnetCollect Project on Videolectures.net
   Mihajela Črnko
   Eurac Research
4. US-Slovenia S&T Cooperation Overview
   Dr. Matej Kovačič
   Embassy of the United States of America

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5. *Dr. Ervin Pfeifer*, 01.06.20, transferred to Department E3*
6. *Matjaž Rihtar, B. Sc., left 01.04.20*
7. Dr. Tanja Zdolšek Draksler

Technical and administrative staff
8. Aleš Buh
9. Mihajela Črnko
10. Ana Fabjan, B. Sc.
11. Adis Krečo, B. Sc.
12. Monika Kropej, B. Sc.
13. Simon Marolt, B. Sc.
14. Davor Orlić, B. Sc.
15. Matija Ovsenek
16. Kim Sevšek, B. Sc.
17. Špela Sitar, B. Sc.

Note:

* part-time JSI member

MILAN ČOPIČ NUCLEAR TRAINING CENTRE ICJT

The mission of the nuclear training centre ICJT is training in the field of nuclear technologies and radiation protection. In addition, ICJT is actively informing the public about those technologies.

Head:
Dr. Igor Jenčič

As in many other areas, the activity of the ICJT was strongly affected by the Covid-19 pandemic. Some training and especially the visits of school groups were conducted using a video-conference system. The premises of ICJT were equipped with numerous hand sanitizers, Plexiglas protection in the lecture rooms, a thermometer for measuring body temperature at the entrance, the number of seats in lecture rooms was reduced and the distance between them increased.

Training in nuclear technologies is our primary mission. We have conducted the *Nuclear Technology* (TJE) course. This course is the first, theoretical phase of training for future control room operators. Due to the Covid-19 pandemic, live lectures were interrupted in March and were replaced by distanced training. Starting on June 1st, and by following all preventive measures, we have continued in the classroom and with exercises on the TRIGA reactor. Due to the lower intensity of the training during the distanced-training phase, the duration of the course was extended by a month and a half.

There were 32 **radiological protection training** courses for the medical, industrial and research use of radioactive sources. Among them was the 6-week initial training for TRIGA radiation department staff (RZ-1) which was for the first time fully performed in Slovenia.

Two **international courses** were organized: one of them in collaboration with the Reactor engineering division and the second one in collaboration with the Reactor physics division and the Reactor infrastructure centre.

Public information remains an important part of our activities. Due to the pandemic, there were significantly fewer physical visits to our information centre, which was in part replaced by lectures and workshops over a video-conference 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 63 groups with a total of 2351 participants this year. Since 1993, there were 189,770 pupils, teachers and others, that visited our information centre. We have continued monitoring and analysing media reports on nuclear energy.

As the activity of the ICJT is strongly related to working with people, we must adopt our mode of operation in the time of the pandemic. The activities were in part conducted by using a video-conference system, while for live lectures the premises and organization of training was modified in accordance with preventive measures.

Figure 1: Radioactivity workshop at the visit of the Slovenian Gymnasium in Klagenfurt am Wörthersee/Celovec, February 2020

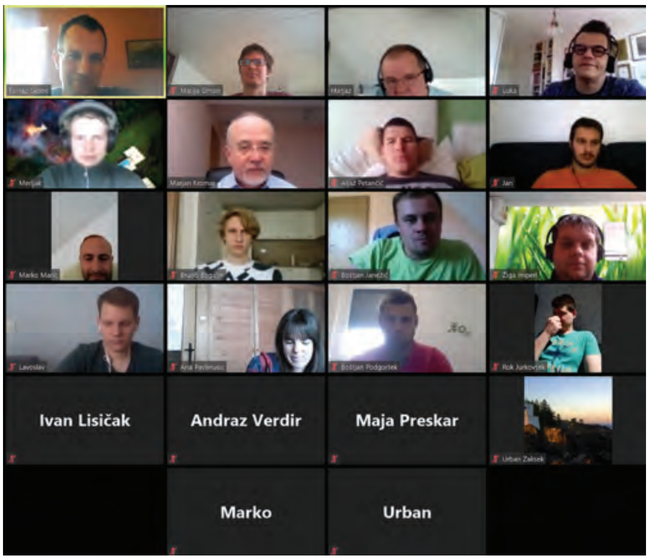

Figure 2: Trainees and lecturers during Zoom session on the Nuclear Technology course

Table of training activities at the Nuclear Training Centre in 2020

Date	Title of the course	Partici-pants	Lecturers	Weeks	Participants × weeks
20.01.-24.01.	Requirements and safety evaluation for NPP SAR	12	9	0.8	9.6
21.01.-12.06.	Radiation protection for RP department staff	1	15	6	6
21.01.-11.08.	Nuclear Technology, Theory	18	16	28	504
09.03.-11.03.	Radiation protection for handheld XRF spectroscopy	9	3	0.6	5.4
09.03.-11.03.	Radiation protection for High Activity Sealed Sources - Refresher Course	1	3	0.6	0.6
09.03.-13.03.	Radiation protection for industrial and other practices (radiography)	3	5	1	3
01.06.	Radiation protection for industrial and other practices	9	3	0.2	1.8
01.06.-2.06.	Radiation protection for industrial and other practices (unsealed sources)	1	4	0.4	0.4
01.06.-4.06.	Radiation protection for Nuclear Medicine Dpt.	10	7	0.8	8
04.06.	Radiation protection for handheld XRF spectroscopy - Refresher course	2	3	0.2	0.4
04.06.	Radiation protection for baggage screening systems - refresher course	4	3	0.2	0.8
04.06.	Radiation protection for industrial and other practices (unsealed sources) - Refresher Course	4	4	0.2	0.8
04.06.	Radiation protection for industrial and other practices	7	3	0.2	1.4
04.06.	Radiation protection for High Activity Sealed Sources - Refresher Course	1	3	0.2	0.2
04.06.-5.06.	Radiation protection for industrial and other practices (radiography) - refresher course	3	3	0.4	1.2
08.06.	Radiation protection for industrial and other practices	15	3	0.2	3
18.06.	Training course for radiation monitoring of public mail	10	1	0.2	2
22.06.	Radiation protection for baggage screening systems	14	2	0.2	2.8
11.08.-20.08.	Radiation protection for RP department staff - refresher course	8	1	1	8
14.09.-15.09.	Radiation protection for Nuclear Medicine Dpt. - Refresher Course	46	4	0.4	18.4
28.09.	Radiation protection for industrial and other practices	4	3	0.2	0.8
28.09.-29.09.	Radiation protection for industrial and other practices (unsealed sources)	5	3	0.4	2
28.09.-01.10.	Radiation protection for Nuclear Medicine Dpt.	2	6	0.8	1.6
28.09.-02.10.	Uppsala University Dedicated Practical Educational Course „Experimental reactor physics“	6	4	1	6
30.09.-01.10.	Radiation protection for workers exposed to radon and thoron	3	4	0.4	1.2
01.10.	Radiation protection for industrial and other practices (unsealed sources) - Refresher Course	7	4	0.2	1.4
01.10.	Radiation protection for handheld XRF spectroscopy - Refresher course	1	3	0.2	0.2
01.10.	Radiation protection for industrial and other practices	7	3	0.2	1.4
01.10.	Radiation protection for High Activity Sealed Sources - Refresher Course	1	3	0.2	0.2
01.10.-02.10.	Radiation protection for industrial and other practices (radiography) - refresher course	3	3	0.4	1.2
05.10.-07.10.	Radiation protection for handheld XRF spectroscopy	6	3	0.6	3.6
05.10.-09.10.	Radiation protection for industrial and other practices (radiography)	3	5	1	3
19.10.	Radiation protection for baggage screening systems - refresher course	7	1	0.2	1.4
20.10.-05.11.	Radiation protection for RP department staff - refresher course	10	1	1	10
26.10.	Radiation protection for baggage screening systems - refresher course	6	1	0.2	1.2
TOTAL		249	142	48.8	613

INTERNATIONAL PROJECTS

1. Training and Tutoring for Experts of the National Regulatory Authorities and their Technical Support Organisations for Developing or Strengthening their Regulatory and Technical Capabilities - MC3.01/13
   Saša Bobič
   Iter-consult Srl - Independent

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. ENRAS: Ensuring Radiation S afety for First Responder Teams in Case of Radiological or Nuclear Accidents
   Matjaž Koželj, M. Sc.
   Government Office for Development and European Cohesion Policy

NEW CONTRACTS

1. Services
   Matejka Južnik, M. Sc.
2. Trainings of the Radiation protection
   Matejka Južnik, M. Sc.
3. Operation of the Nuclear Information Centre in 2020
   Dr. Igor Jenčič
   Gen energija, d.o.o.
4. Basic Training Course on Nuclear Technology and Nuclear Power Plants
   Dr. Igor Jenčič
5. ICJT Training Programme implementation in the year 2020
   Dr. Igor Jenčič
   Nuklearna Elektrarna Krško d. o. o.

STAFF

Researcher
1. **Dr. Igor Jenčič, Head**

Technical officers
2. *Bojan Ambrožič, B. Sc., left 15.01.20*
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.

Figure 3: Training session in the control room of the TRIGA research reactor

Figure 4: Trainees in the lecture room during the Nuclear Technology course, June 2020

Figure 5: Group photograph of trainees and lecturers at the closure of the Nuclear Technology course

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ORIGINAL ARTICLE

1. Marko Soderžnik, Bojan Ambrožič, Kristina Žagar, Matic Korent, "Limits of grain boundary engineering in nanocrystalline Nd-Fe-B melt-spun ribbons", *Materials letters*, 2020, **264**, 127338.

PUBLISHED CONFERENCE CONTRIBUTION

1. Matjaž Koželj, Vesna Slapar Borišek, Radko Istenič, "Practical demonstrations - key to efficient explanations of radioactivity to pupils and students", In: *ANIMMA 2019, Advancements in Nuclear Instrumentation Measurement Methods and their Applications, June 17-21, 2019, Portorož, Slovenia*, Proceedings, (EPJ Web of Conferences **225**), EDP Sciences, 2020, 10001.
2. Matjaž Koželj, Vesna Slapar Borišek, "The possibility for distant training and examination in radiation protection in Slovenia", In: *NENE 2020, 29th International Conference Nuclear Energy for New Europe, September 7-10, Portorož, Slovenia*, Proceedings, Nuclear Society of Slovenia, 2020, 1601.
3. Tomaž Skobe, "Distance nuclear training", In: *NENE 2020, 29th International Conference Nuclear Energy for New Europe, September 7-10, Portorož, Slovenia*, Proceedings, Nuclear Society of Slovenia, 2020, 1602.
4. Radko Istenič, Igor Jenčič, "Public opinion about nuclear energy - year 2020 poll", In: *NENE 2020, 29th International Conference Nuclear Energy for New Europe, September 7-10, Portorož, Slovenia*, Proceedings, Nuclear Society of Slovenia, 2020, 1701.

THESES AND MENTORING

1. Bojan Ambrožič, *In situ synthesis and growth of nanoparticles using a liquid cell transmission electron microscopy:* doctoral dissertation, Ljubljana, 2020 (mentor Sašo Šturm).

RADIATION PROTECTION UNIT

SVPIS

SVPIS has been involved in ionizing-radiation measurements and radiation protection since the commissioning of the TRIGA MARK II Research reactor in 1966. The responsibility of SVPIS is the radiation control of all the activities at the Institute dealing with ionizing radiation. Our main task is the supervision of work in the reactor with the Hot Cell Facility and we are authorised by the regulatory authority to perform environmental monitoring.

SVPIS also controls 17 laboratories that use sources of ionising radiation in their research work. There are different sources of radiation used, such as sealed sources, open sources, X-ray units and the accelerator TANDETRON, which need regulatory control. Furthermore, we are involved in radioactive-waste management.

SVPIS is authorized by the Slovenian radiation protection administration and nuclear-safety administration to perform control in industrial and research institutions dealing with open or sealed radioactive sources and X-ray units.

The measurements of dose rate, contamination and gamma spectrometry are performed by an accredited method (LP-022, EN ISO/IEC 17025). In this year, we expanded the accreditation to radon-concentration measurements.

Head:
Matjaž Stepišnik, M. Sc.

Personal dosimetry

Personal doses of 125 workers that regularly or occasionally deal with ionizing radiation were monitored with Thermo Luminescent Dosimeters. The maximum individual yearly dose was 0.36 mSv. This is only 1.8 % of the regulatory limit for occupational exposure (20 mSv per year) and 36 % of the limit for the public (1 mSv per year). The collective dose at JSI in the year 2020 was 2.9 man-mSv.

Supervision of research reactor and laboratories

The controlled area of the Research reactor, the Hot Cell Facility and the Department of Environmental Sciences was monitored on a weekly basis. During some activities, the constant presence of a radiation-protection worker was needed (i.e., for the opening of activated samples or radioactive-waste management). Measurements of dose rate, surface contamination, contamination of different objects and personal contamination were performed routinely. In most cases, no or very low contamination levels could be measured. Locally elevated radiation levels could be measured mostly in the reactor's controlled area.

At present, 106 sources of radiation are in use, which require regulatory control and additionally 458 low-activity sources in different laboratories.

In 2019, 20 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 program. The program consists of effluent measurements and measurements of samples in the environment. Activity concentrations of gamma emitters in water samples, filters, noble gases, soil samples and sediment samples were measured periodically. About 500 different samples for the reactor and different laboratories were measured with gamma spectrometry. Environmental passive dosimeters were used to monitor radiation levels in the surroundings of the reactor. Based on the effluent measurements and a conservative environmental transfer model, the effective dose to the reference group of the public was estimated to be less than 1 μSv/year. In 2020 the exposure of the public due to activities at the Reactor Center was insignificant.

Expert assessments and measurements for outside customers

The Radiation Protection Unit is authorized for the 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 46). Our group has participated in the evaluation of radiological monitoring of the Krško NPP, research reactor TRIGA and storage for low- and intermediate-level waste in Brinje.

STAFF

Technical officers
1. Dr. Tinkara Bučar
2. **Matjaž Stepišnik, M. Sc., Head**

Technical and administrative staff
3. Thomas Breznik, B. Sc.
4. Tanja Murn, B. Sc.
5. Nina Udir, B. Sc.

BIBLIOGRAPHY

Independent Component Part or a Chapter in a Monograph

1. Matjaž Stepišnik, "Radioaktivnost v rečni vodi, sedimentih in ribah", In: *Ugotavljanje stopnje radioaktivnosti v okolju zaradi nadzorovanih izpustov iz NEK*, Institut Jožef Stefan, 2020, 108-1-108-19.

CENTER FOR TECHNOLOGY TRANSFER AND INNOVATION CTT

The Technology Transfer Office was established in 1996 and transformed in January 2011, when an independent Centre 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 with finding suitable local and international research partners for contract and collaborative research. We also support transfer knowledge from science to the school system and promote recognition of the JSI, and science in general, among young people and the wider population.

Head:
Dr. Špela Stres, MBA, LLM

The Centre's success is based on 13 professionals, 6 of who 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). 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, and three team members hold the US "Certified Licensing Professional" certificate .

Our essential tool is a created network of contacts with enterprises and other organizations in Slovenia and abroad. **Our services**, fine-tuned to 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 have also procured our services in 2020.

Figure 1: Winners of the Prize for best innovations from public research organizations (photo: M. Verč)

In 2020, CTT faced several activity-related **challenges**, the biggest of which were:

(i) the content-based upgrade of financial consulting for SME-PRO collaboration;
(ii) the Innovation fund (Proof-of-Concept) call at JSI,
(iii) the systematic professionalization of a position in the field of technology transfer.

In 2020 we unified our support to SMEs seeking funding for collaborating with researchers, particularly in an income-tax deduction. In 2020 we spearheaded the Proof-of-Concept Innovation Fund initiative, consolidated the guidelines on managing the Fund, and implemented the call, resulting in funding for six successful JSI research projects to increase their technology TRL. In 2020 we introduced, for the first time, a 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.

Marketing of 27 JSI technologies, 153 identified RR topics. Sixteen licenses and 31 research and development agreements signed with companies, domestic and foreign contracts representing 7 and 31 %, respectively, of the cash flow at JSI.

Despite the epidemiological situation in 2020, we managed to perform our services thoroughly and without significant obstacles. We organized the International Technology Transfer Conference, which took place online and organized company visits and school visits in the same manner. In 2020 we agreed to join a consortium of digital innovation hubs in Slovenia within the eDIH network. We joined an application for carrying out the JSI Infrastructure Programme in the period 2022–2027.

In 2020 the Centre for Technology Transfer and Innovation was partly funded through **two larger and five smaller European and national projects**. Projects were run under various funding programmes and schemes. These included Enterprise Europe Network (EEN) Slovenia (COSME scheme), EEN We4SMESLO, and KET4Clean Production (Horizon 2020), SYNERGY and KETGATE (INTERREG Central Europe), and Co-Create (INTERREG MED) as well as the national project KTT (MIZŠ). Project activities were combining and completing our core TT activities. Within the KTT project, we coordinate the Consortium for technology transfer from PRO 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 mutually interact with, and complement, each other.

GROUP FOR PROTECTION AND MARKETING OF INTELLECTUAL PROPERTY processes **IP protection and marketing** cases that are submitted through the single entry point following introductory meetings with researchers (33), prepares patentability assessments, including in-depth state-of-the-art analyses (19). The Group also conducts detailed market potential analyses (14), helps develop the invention description for disclosure within the Institute (19), helps fulfil the terms for patent application filing (14), prepares agreements on ownership of intellectual property (6), searches for suitable patent attorneys for filing and processing the applications (20), and advises about the strategy of international (13) and national (7) expansion of patent protection. The Group also carries out (i) passive marketing: 27 technology profiles promoted through the Enterprise Europe Network, 65 expressions of interests received, and (ii) active marketing: technologies above promoted directly to more than 200 companies and other organizations, with 12 expressions of interests received. Moreover, Group members arrange to sign non-disclosure agreements (13), take part in negotiations (22), and prepare and close license (15) and research and development (18) agreements, while having a support role in 5 additional contracts.

Organization of the 13th International Technology Transfer Conference. More than 120 visitors. The competition for the best innovation; two ITTC best innovation awards, two WIPO awards – 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.

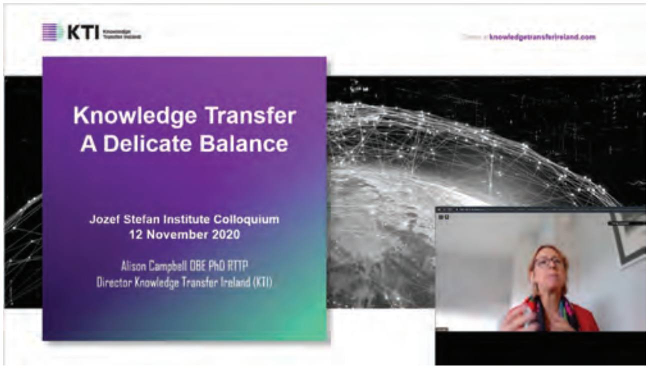

Figure 2: Online Colloquium: dr. Alison Campbell - Knowledge Transfer - A Delicate Balance

Group members also provided individual consulting regarding all phases of **spin-out** company creation (6). They helped with the preparation of business plans (3), manage discussions on the arrangement of the relationship between the JSI and the researcher (1), prepare documentation for spin-out creation (1), prepare agreements for access to infrastructure (2), and prepare license agreements (1) for the use of technology within the spin-out company.

The Group also prepared the **Proof-of-Concept Innovation Fund** initiative, consolidated the guidelines on managing the Fund, and implemented the call, resulting in funding for six successful JSI research projects to increase the TRL.

GROUP FOR PROMOTION, EDUCATION AND PROJECT MANAGEMENT

To **encourage researches** 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 2020, six teams applied – 2 from JSI, 3 from more than one PRO, and 1 from another PRO. At the 13th International Conference on Technology Transfer, a ceremony for awarding the two best innovations took place. In addition, at the Conference, for the first time, two WIPO awards were given: a 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. JSI researchers were also assisted in presenting their innovations at the ARCA 2020 international fair in Zagreb, winning the gold and silver medal, and attending the virtual Fair on innovation and entrepreneurship Sarajevo 2020 innovation-of-the-year, and the silver medal awards.

Collaboration within the DG Research & Innovation in the European Innovation Council Management Group. We collaborate with the United Nations, as members of the 10-Member Group for support of the Technology Facilitation Mechanism (10MG TFM) and with the World Intellectual Property Organization (WIPO) in the context of their international worldwide activities. We act as chair of the BioChemTech Group in the Enterprise Europe Network and preside over the Expert council of independent centres at JSI, and the Association of Technology Transfer Experts of Slovenia.

The Group **informed** 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) and foreign partner searches (35), and helped write project applications, especially in the "Exploitation" and "Dissemination" parts. They disseminated information to TT coordinators weekly, which has efficiently contributed to the submission of new projects with new international partners (24; 11 with JSI). We also published several articles in Slovenian journals (9).

Among notable **events**, the group planned the annual Open Day at JSI (having been cancelled due to the pandemic), organized school visits at JSI (20). They carried out an entrepreneurial education session for young researchers (1 session, 25 participants) and organized the 13th International Technology Transfer Conference with more than 120 participants. The group also organized an advisory visit to the MIZŠ and MGRT ministries, SID bank and SVRK agency, by the distinguished international expert in technology transfer, Dr Alison Campbell.

The Group issued several **publications** – compiled and edited a 550-page brochure on Patents from the Jožef Stefan Institute between 1998 and 2018, designed a compendium on technology transfer for the Slovenian economy and science, and a manual on business support environment, with the emphasis on problems in technology transfer, directed primarily toward Slovenian policymakers. The group also published three informational leaflets on CTT services and re-issued manuals on technology transfer, opportunities for collaboration, and development opportunities at the Jožef Stefan Institute.

Figure 3: Publication Patents of the Jožef Stefan Institute 1999-2018

GROUP FOR CONTRACTUAL COLLABORATION WITH INDUSTRY visits both large and small companies (33 in 2020), organizes their return visits to the JSI (18), organizes sectorial and regional tours of companies to the JSI (virtual visits as of the onset of the pandemic), and collaborates with other entities of the support environment. This Group's members regularly find new topics for cooperation within the development projects amongst companies and researchers (153), 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 2020, 26 international agreements on long-term collaboration, were signed. The Group also helped sign license (1) and R&D (3) agreements and supported five additional contracts.

The Groups mentioned above work closely together to **passively market** technology and business profiles (53) in the Enterprise Europe Network global base, and coordinate the market interests (134) for SMEs (111) and researchers (23), and create expressions of interests to foreign published profiles (115) for businesses (75) and researchers (40). The Groups co-organized 11 **international B2B events** with 76 Slovenian SMEs and researchers who conducted 180 meetings with a foreign partner.

In 2020, the three Groups jointly helped close 16 license and 31 research-and-development contracts with 19 different organizations. The activities of the CTT have increased significantly in the area of contracting over the last year, having represented 7 % of the JSI cash flow due to domestic, and 31 % due to international contracts.

- **Proof-of-Concept Innovation Fund call, funding for six JSI research projects for increasing the technology TRL, originating from direct revenue from license fees in the amount of €45,000**
- **Milestone of 300 introductory meetings with companies (since the establishment of CTT).**
- **12th award ceremony for the best innovation with market potential; more than €56,000 awarded in total since the first International Technology Transfer Conference.**
- **JSI researchers informed more than 200 relevant domestic and international project calls**
- **JSI researchers informed about, and assisted in, applying to domestic and international competitions, winning 6 awards.**
- **Introduction of a section on research in technology transfer at the International Technology Transfer Conference, thereby raising the context of technology transfer to a level of scientific discourse.**

GROUP FOR INNOVATION RESEARCH

We operate as **evaluators and external experts** in Slovenia and the European Commission›s frame for different respected international institutions (EC ERC, EUREKA, RRI). We were recognized by the JRC as one of the most propulsive technology-transfer offices in the EU and were included into the **TTO Circle**, the Group of PROs most active in the field of knowledge and technology transfer (including the institutes Max Planck, Weitzman, Fraunhofer, VITO, and VTT). We collaborate with the **United Nations**, as members of the 10-member Group for support of the Technology Facilitation Mechanism (10MG TFM), and with the **World Intellectual Property Organization** (WIPO) in the context of their international worldwide activities, having given several talks within their training cycles, for example, in Belarus and Latvia. We are members of the Expert Group **DG Research & Innovation in the European Innovation Council**. In 2020 we continued our membership within the BioChemTech, Materials, and ICT **Sector Groups within the Enterprise Europe Network**, wherein we hold the chairmanship of the BioChemTech Group. We furthermore preside over the Expert council of independent centres at the JSI, the Association of Technology Transfer Experts of Slovenia, and the Committee for spin-out companies at JSI.

Organization of Conferences, Congresses and Meetings

1. Co-Create project workshop: Use of Gamification for Reaching Goals, JSI, Ljubljana, Slovenia, 30.1.2020

2. SYNERGY project workshop: Simulated Crowdfunding, JSI, Ljubljana, Slovenia, 13.2.2020
3. 13. International Technology Transfer Conference, 13.ITTC; online, 8.10.2020
4. SYNERGY project workshop: Simulated Crowd Innovation Day, online, 16.10.2020
5. JSI Colloquium: Knowledge Transfer – A Delicate Balance; online, 12.11.2020
6. Meeting with dr. Alison Campbell, Knowledge Transfer Ireland, and representatives from Ministries for Education, Science and Sport (MIZŠ) and Economic Development and Technology (MGRT), the Government Office for Development and European Cohesion Policy (SVRK), and the Slovenian Promotional Development and Export Bank (SID); online, 12.-13.11.2020
7. Young Hopes 2020 – Entrepreneurial and innovation workshop for young researchers; online, 13.11.2020

INTERNATIONAL PROJECTS

1. COSME-EEN-SGA4 - EEN Slovenia 4; EEN Slovenia Services in Support of Business and Innovation in Slovenia
   Dr. Špela Stres
   European Commission
2. 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
3. H2020 - We4SMESLO 5; Enhancing Innovation Management Capacity in Slovenian SMEs by EEN Slovenia
   Dr. Špela Stres
   European Commission

R&D GRANTS AND CONTRACTS

1. Co-Create: Setting up a network of COmpetitive MED Clusters with the contribution of cREATive Industries
   Dr. Špela Stres
   Joint Technical Secretariat Med Programme
2. Central European SME Gateway zo Key-enabling Technology Infrastructures - Sparking new Transnational KET Innovation Ecosystem
   Dr. Špela Stres
   Bay Zoltan Alkalmazott Kutatasi Kozhasznu
3. Synergic Networking for Innovativeness Enhancement of central european actoRs focused on hiGh-tech industry
   Dr. Špela Stres
   Interreg Central Europe Programme
4. The consortium for technology transfer from the PRO to the economy
   Dr. Špela Stres
   Ministry of Education, Science and Sport
5. JSI Share of License Revenues related to Exploitation of Inventions - Abroad (JSI License Revenue Share - Abroad)
   Dr. Špela Stres

STAFF

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Technical officers
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5. Dr. Duško Odić
6. Dr. Levin Pal
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8. Marjeta Trobec, M. Sc.

Technical and administrative staff
9. *Dr. Zdravko Balorda, left 01.09.20*
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11. Matej Mrak, B. Sc.
12. Urška Mrgole, B. Sc.
13. Miha Pitako, B. Sc.
14. Robert Premk, B. Sc.

BIBLIOGRAPHY

Published Conference Contribution (invited lecture)

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5. Levin Pal, "The awareness on environmental protection issues as reflected through the inventions", In: *13. ITTC, 13th International Technology Transfer Conference, 8 October 2020, Ljubljana, Slovenia*, Proceedings of the 23rd International Multiconference Information Society (IS 2020), volume E, Institut "Jožef Stefan", 2020, 53-59.
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1. Angelos Dennis Keromytis, Jes Broeng, Julien Chiaroni, Carsten Dreher, Fiona Murray, Marie-Elisabeth Rusling, Špela Stres, "Recommendatins & guiding principles: programme creation", In: *Implementing the pro-active management of the EIC pathfinder for breakthrough technologies & innovations: lessons from the ARPA model & other international practices*, European commission, 2020, 20-43.
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3. Cheryl Martin, Jes Broeng, Julien Chiaroni, Franz-Werner Haas, Fiona Murray, Marie-Elisabeth Rusling, Špela Stres, "Recommendatins & guiding principles: transition activities", In: *Implementing the pro-active management of the EIC pathfinder for breakthrough technologies & innovations: lessons from the ARPA model & other international practices*, European commission, 2020, 53-73.

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1. Špela Stres, Levin Pal, *Priročnik o prenosu tehnologij: za slovensko gospodarstvo in slovensko znanost*, Center za prenos tehnologij in inovacij na Institutu Jožef Stefan, 2020.

CENTER FOR SMART CITIES AND COMMUNITIES CSC&C

The Center for Smart Cities and Communities (CSC&C) was established at the beginning of 2017. On 1 January 2019, 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 Innovation Partnership Smart Cities and Communities

Strategic Development Innovation Partnership Smart Cities and Communities is a partnership in which stakeholders have joined forces in developing and selling solutions to raise the quality of life in the cities of the future.

The purpose of SRIP SC&C is to connect companies and research institutions in a particular field into value chains, to set priorities for development investments and to coordinate R&D activities. We are building a good support 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 analysis, human-resources development, intellectual-property protection and internationalization.

We want to approach the smaller towns in Central and Eastern Europe with solutions, as we consider that due to its size and geostrategic position, Slovenia is very suitable as a reference country for various "smart urban" solutions suitable for implementation in other parts of Central and Eastern Europe. SRIP SC&C was formally constituted at the Assembly on 23 March 2017, and currently involves more than 120 companies and research institutions from all over Slovenia.

Key areas and technologies

Strategic Research and Innovation Partnership Smart Cities and Communities covers several research areas as well as the ICT horizontal key enabling technologies (Figure 1).

SRIP SC&C creates and supports business and research synergies in smart cities for new products, services and technologies, and helps companies enter the global market by focusing on niche areas, with the aim of making Slovenian companies an important European provider of such solutions.

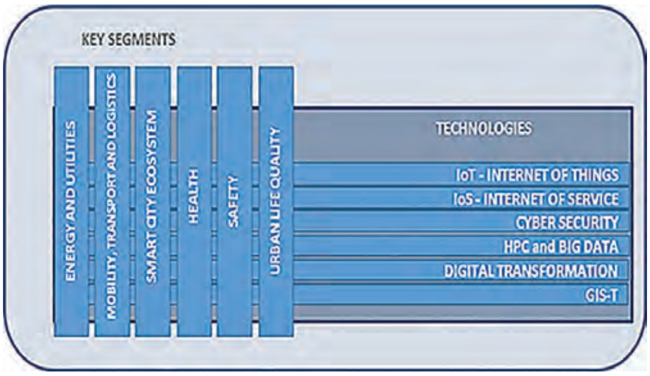

Figure 1: Key areas and technologies

The partnership includes the current contents of the new 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 has identified the importance of carbon-neutral smart cities as one of the five key areas.

Partnership goals:

- creates and supports 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 in the 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);
- promotion of members and their products and services;
- direct information to the SRIP SC&C members;
- improving the quality of life in cities and communities: collaboration with municipalities, cities.

In 2020 we successfully completed the second phase of the SRIP SC&C Operation and signed an agreement with the Ministry of Economic Development and Technology (MGRT) on co-financing the third phase of the operation "Strategic Development Innovation Partnership in Smart Cities and Communities", which confirms the SRIP SC&C guidelines set out in Action Plans. At the end of 2020, the Government Office for Development and European Cohesion Policy (SVRK) approved the extension of SRIP Operations, which for us means co-financing SRIP SC&C

until 30 September 2023. Since the Covid-19 pandemic began in March 2020, we adapted our operations to the situation and conducted most events and meetings virtually.

Activities within the Organizational Structure of SRIP SC&C

At the beginning of the year we paid the most attention to the amendment of the Action Plan and preparations for the submission of the application for the third phase of the SRIP SC&C Operation. On 13 February 2020, at sessions of the SRIP SC&C Steering Committee and Program Board, we adopted the Action Plan 2020–2022 and the Work Program for the third phase of the SRIP SC&C Operation. On 14 February 2020 we applied for the third phase of the SRIP SC&C Operation.

With the start of the third phase of the SRIP SC&C Operation we focused more intensively on the implementation of the activities of the renewed SRIP SC&C Action Plan. At the seventh session of the SRIP SC&C Program Board, on 21 May 2020 we presented a summary of the Action Plans for Vertical and Horizontal SRIP PMiS with examples of good practices and held elections of members of the Program Board Presidency. On 4 June 2020, at the third Assembly of SRIP SC&C, we presented the amendments to the Rules of Procedure of SRIP SC&C, the Report on activities performed in 2019 and held elections of members of the SRIP SC&C Steering Committee. At the sixth session of the SRIP SC&C Steering Committee, on 12 November 2020, a new President of the Steering Committee was appointed by the Chamber of Commerce and Industry of Slovenia. The Steering Committee has a domain for the financial aspects of SRIP SC&C. The members were also acquainted with the activities of the third phase of the SRIP SC&C Operation and the guidelines for the Business Plan for 2021.

The eighth session of the SRIP SC&C Program Board, on 18 December 2020, was intended to acquaint with the activities in the field of renewal of the S4 Smart Specialization Strategy and guidelines regarding the SRIP SC&C activities after 2022.

Cooperation between SRIPs and Ministries

In the second half of the year, in cooperation with SVRK, all SRIPs prepared a draft document of the renewed S4 Smart Specialization Strategy. We focused on Criterion 4: The Enterprise Discovery Process (EDP) and the related revised definition of focus areas and related products. During this period, meetings were held with individual verticals and horizontals, as well as with other SRIPs, to focus and define potentially related and complementary areas of activity.

Throughout 2020, meetings of the Working Group of SRIP Coordinators were held. The basic direction we follow is the connection of partners within individual SRIPs and between SRIPs, with an emphasis on connecting the economy, knowledge institutions and the state. We participated in the formulation of the Slovenian Industrial Strategy. In 2020, our meetings focused on reviewing the state and further activities of the S4 renovation, in cooperation with MGRT, Ministry of Education, Science and Sport (MIZŠ) and SVRK.

On 14 September 2020 a workshop on smart specialization in Slovenia was held within the Interreg A-RING project, with the aim of informing about the state of activities in the field of renewal of the S4 Strategy by SVRK. The workshop was attended by all SRIPs.

Cooperation with other Institutions

In the framework of cooperation with other institutions, we paid great attention to cooperation with municipalities in the preparations for the MPA tender, on the topic of IoT solutions for cities and municipalities. In the catalogue of digital solutions for smart cities and communities, we collected the activities and products of SRIP SC&C members for MPA. In the municipality of Grosuplje, we organized a presentation of IoT services and products of our members. We have established a connection between our members who have service products and the cities-municipalities that need these services. We conducted a series of coordination meetings with North Primorska municipalities and gained a set of priority areas and invited SRIP SC&C members to engage with their products and services by completing the survey. At the MPA, we submitted the Draft Strategy for "Smart Cities" for the period 2020–2024, prepared by a member of SRIP SC&C, Municipality of Krško.

SRIP SC&C is involved in the preparation of the document "National Program for Promoting the Development and Use of Artificial Intelligence in the Republic of Slovenia until 2025", which is being prepared jointly with the Information Society and Informatics Directorate at the Ministry of Public Administration and in cooperation with key stakeholders in Slovenia. Under the European Green Agreement, the SRIP SC&C is involved in activities related to the initiative: "100 climate-neutral cities by 2030", in line with the Mission's financial instrument. In cooperation with the representatives of the Technology Park, preparations are underway for the event within the framework of the EU Presidency in Slovenia.

Free workshops and seminars for SRIP SC&C members

We organized free online workshops and activities for SRIP SC&C members: 14 October 2020: Tetramax: User interface design-practical guidelines, online workshop; 25 November 2020: Tetramax: Embedded systems with FPGA circuits, online workshop. In cooperation with the expert group from UL FRI, we are preparing the open-source online Platform SRIP SC&C: Solution Market and Technology Casino. We have established a membership with the EIP-SCC, which has the strong support of the European Commission and an important role in bringing together cities, industries, investors, researchers and other smart city actors.

As part of **promotion and internationalization**, we participated in high-profile events in Slovenia and abroad: Partnership in the DEAS project - Data Economy as a source of cooperation, competitiveness and new services in the Alps; 23–24 September 2020: Co-organization of the International Conference "Living bits and things 2020", presentation of SRIP SC&C; 4 November 2020: Expo 2020 Dubai, as part of the virtual Pre Expo events, a presentation of Slovenia and Operation SRIP SC&C took place; 10 December 2020: Section Slovenian Association for Energy Economics, presentation of SRIP SC&C projects and activities within the SAEE.

In the field of **informing the public** about the operation and vision of the SRIP SC&C partnership, articles were published in "Eko Dežela" magazine (November 2020) regarding digitalization and the concept of smart villages and towns in the Republic of Slovenia and an article in the newspaper DELO (15 May 2020) entitled "The concept of a city that will no longer be only smart but also safe after the epidemic." In November, we gave an interview for Radio "Rai Furlanija Julijska Krajina", Trieste, Studio D show, entitled "Smart through the city". On the SRIP SC&C website, we regularly publish news and events for members.

R&D GRANTS AND CONTRACTS

1. Strategic Research & Innovation Partnership Factories of the Future (SRIP PMIS)
   Dr. Nevenka Cukjati
   Ministry of Economic Development and Technology
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. SI4CARE
   Dr. Nevenka Cukjati
   Ministry of Economic Development and Technology
4. Support for Strategic Research and Innovation Partnerships (SRIP) and Priority Areas of Smart Specialization (SRIP PMiS)
   Dr. Nevenka Cukjati

STAFF

Technical and administrative staff

1. **Dr. Nevenka Cukjati, Head**
2. Petra Hauschild, B. Sc.
3. Mojca Kristl, B. Sc.
4. *Željka Kukec, B. Sc., left 01.04.20*
5. *Tjaša Lazič, B. Sc., left 27.04.20*

CENTER FACTORIES OF THE FUTURE CFoF

Centre Factories of the Future - CToP, run by Rudi Panjtar, was established in early 2017. The main task of the newly established centre is to coordinate and operate the Strategic Development and Innovation Partnership of Factory of the Future (SRIP ToP). In addition, the centre 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 in the coming years.

Head:
Rudi Panjtar , B. Sc.

What does the Factory of the Future Strategic Development Innovation Partnership offer?

The SRIP Factory of the Future (SRIP ToP) strategy is to gather and integrate Slovenian research and innovation knowledge and experience in the industrial and academic spheres and highlight the priority breakthroughs of new products, technologies and services for Factories of the Future. We have established a supportive environment with expert services for industry and research organizations, with an emphasis on developing new cutting-edge technologies that combine and build on existing Slovenian research and innovation achievements.

The key functions of the strategic, long-term interconnectivity are the definition and supplementation of the strategic action plan in the field of Factories of the Future, activities in scope of the development of joint services, internationalization, development of human resources, representation of joint interests towards the state, etc. Part of the services will be done in cooperation with other institutions.

SRIP ToP **creates and supports** business and research synergies in the area of future factories for new products, services and technologies, and helps businesses enter the global market by focusing on niche areas.

The 95 members of SRIP ToP come from various companies, associations or institutions from Slovenia. The operation of SRIP ToP focuses on the greater integration of knowledge and the joint appearance of stakeholders in domestic and foreign markets. The primary goals are to increase the share of high-tech industrial products in exports and to increase the added value of Slovenian industry.

Key areas of activity

The SRIP Factories of the Future includes eight areas (verticals), and horizontal networks with key technologies that are interwoven (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 ToP also indirectly contributes to accelerating the transition to a low-energy, energy-efficient economy, reducing greenhouse-gas emissions, and to intensively promote the transition to a low-carbon society and to a circular economy. The essence of the concept of factories of the future is mainly reflected in the greater potential for the reuse of raw materials, made possible by more flexible and optimally managed production.

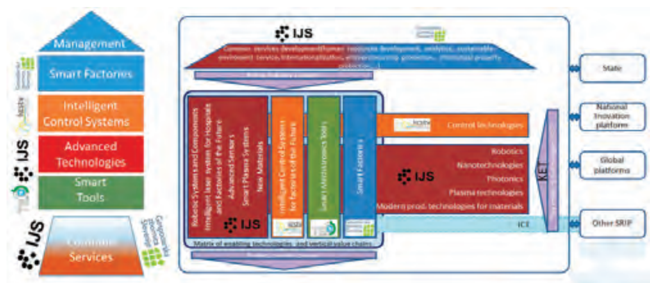

Figure 1: Scheme of SRIP ToP domains

In the field of internationalization, we actively participated with the Directorate for economic and public diplomacy of the Ministry of Foreign Affairs, which is preparing for EU presidency, where they also plan to highlight some of the topics in our field.

We joined the influential WMF (Word Manufacturing Forum) and SPIRE (Sustainable Process Industry through Resource and Energy Efficiency). In the field of robotics, we have joined the RIA (Robotics Industries Association), with which we ambitiously enter markets outside the EU.

We continued our activity in the Vanguard Initiative, especially in the field of virtual factory and 3D printing, where we became full members of the smaller groups, working in the scope of the mentioned pilots.

In the EU S3 platform, as part of the modernization of production, we are the co-leading partner for artficial intelligence in production (AI-HMI) and the leading partner for the implementation of Industry 4.0. We also actively represent our members in the preparation of the Slovenian strategy of artificial intelligence and we were also among the initiators of the establishment of the AI4SI association. As part of AI-HMI, we are designing an interregional laboratory for AR / VR, cooperating robots and a smart factory.

In the field of artistic information, cooperation with BDVA (Big Data Value Association) is also assumed, where we will cooperate in the field of using AI in big data in production.

We have established cooperation with the photon cluster ALFA-RLH, with which we are planning to sign a cooperation agreement.

During the year, CToP intensified its cooperation with international partnerships, where we participated in joint applications for three projects under Horizon 2020 and Cosme (European Agency for Small and Medium-sized Enterprises) and also with the EU Covid 19 Horizon 2020 call. Although the project applications from international consortia were highly rated, we were not successful with the application due to the high competitiveness of the European Union calls. However, as a result CToP has established important alliances with strong industrial networks and partners from all over Europe (such as AFIL Lombardy Smart Factory Association, ALPHA-RLH-cluster in the field of photonics and microwaves from France, EIT Manufacturing, etc.). In 2020, we approached the preparation of cooperation agreements with some of them and/or started applying for a new strategic project for the cooperation of major European industrial clusters to accelerate the transition of European SMEs to Industry 4.0. Thus, as part of the Horizon Innosup call, aimed at connecting European clusters, we prepared and applied for a new major project of industrial cluster cooperation with the expected start of cooperation in the second half of 2021, if the application is successful. CToP was also successful in the Horizon Innosup tender for the development of new, specialized knowledge of innovation systems with the Go Dip project, where we are the leading partner. HIT - Hub Innovazione Trentino from Italy and INNOSQUARE innovation platform from Friborg, Switzerland are also participating partners in the project. The Go Dip project is aimed at building specialized consulting activities of partners in the field of digital intellectual-property-rights management and the monetization of the digital data of companies through the valorization of digital assets as a strategic underused capital of digital companies. The project will start in March 2021. The total value of the project is €50,000, of which €18,000 is funding for CToP.

At the end of the year, CToP was invited by the Government of the Republic of Slovenia (Ministry of Foreign Affairs) to participate as an active member in Action Group 2 in the field of macro-regional economic development, which provides strategic guidance to the Alpine macro-region for investment in R&D, digital industry of the future and i4.0 industry. The group provides a basis for planning the European Union's new financial programmes in the field of European territorial, industrial, research and environmental policies.

To intensify the internationalization of CToP and members of the SRIP FoF, we have also identified a number of new financial and research and development platforms and measures within the programmes of NATO, the European Space Agency and major European and global research infrastructures and networks such as, e.g., RIA in the field of robotics and the European Platform for Bioeconomy and many others, benefiting the know-how of the CtoP and members of the SRIP FoF.

Last year- we successfully completed the 2nd phase of the SRIP Factory of the Future project and moved on to the 3rd phase of the project, where we will further intensify and focus our activities. Last year was special, as it was marked by several things that greatly influenced our operations, including the COVID-19 epidemic and its related measures both home and abroad, and the application for the 3rd phase of the SRIP Factory of the Future project with an ambitious action plan.

According to the action plan, we have established all the processes for the operation of the internal organization - the establishment of four clusters, coordination and business model between clusters, and the establishment of a network of vertical value chains with horizontal networks' coordinators.

We have established cooperation with the Pomurje Technology Park, with which we plan to cooperate in projects related to Industry 4.0 and robotics.

We co-organized KOC 3.0 Factories of the Future, where we enabled the maximum involvement of our members and prepared, together with other partners, a varied and interesting training programme. We established a connection between KOC - Factories of the Future, the Munera programme and the development of human resources within the SRIP ToP, and accepted a commitment to joint cooperation in the field of human resources. We also participated in the tender for KOC DM, where we look to bring our members (both companies and research organizations) closer to management skills and processes for the implementation of sustainable design.

We prepared an action plan for the 3rd phase of the SRIP operation, where through projects proposed by our industry members we made changes and adjustments to key areas of activity and directions of development that will have a major impact on domestic calls in the next 3 years and the preparation of operational programmes in the fields of economy and science.

We also participated in the preparation of proposals for "corona measures", where we tried to encourage greater state assistance in investing in new technologies, digitalization and automation.

We have established cooperation with other SRIPs, 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 discussions and preparations of operational programmes for the next financial period.

In cooperation with SVRK, in the process of entrepreneurial discovery, we made changes in certain product and development areas, which will be included in the renewed smart specialization strategy for the period 2021-2027. We put the integration of key technologies in the forefront, the development and financing of which is crucial for the success of the entire Slovenian smart specialization.

We conducted SRIP FoF presentations at various events and presented SRIP FoF and our activities at various meetings both home and abroad.

We have renewed our website, which is becoming an increasingly popular contact point for news in the field of technology and our activities, and in combination with social networks, it is acquainting an ever-widening circle of followers with our activity. We have updated and enriched our weekly news, which reaches a nice readership among the recipients.

The period of the epidemic and governmental change has severely affected our direct activities, which we planned for members in 2020. The period of contracts invalidity also stopped the financing of external and internal service providers. During this time, we have applied for several EU tenders, the results of which we are still waiting for.

As part of the preparation of the action plan and with the aim of promoting networking, the exchange of information and encouraging organizations to join the SRIP FoF, in 2020 we conducted several presentation events of the SRIP FoF. Among the most resounding were: organization and implementation of an international two-day workshop Nanotechnology and nanoApplication Workshop, IFAM fair, presence at the First Technological Breakfast, co-organized by SRIP FoF together with the Slovenian Chamber of Commerce, resounding presentation of breakthrough companies to EU regions in Brussels. Since March, most events have been cancelled due to poor epidemiological conditions, during which time most events have moved online. Thus, we have prepared a very successful online event Counterfeiting - How to insure and take action, which was created in cooperation with the Financial Administration of the Republic of Slovenia, the Office of the Republic of Slovenia for Intellectual Property and the Association of Slovenian Intellectual Property Representatives.

We are further developing the connection we have established with KOC-TOP, giving our members access to workshops and conferences organized by KOC-ToP. We also organized the first practical "hands-on" workshop, where students were introduced to the theory and practice of using digital twins in the environment of the Demo Center - Smart Factory at the Faculty of Mechanical Engineering.

Talks are underway with the coordinators of individual vertical value chains and horizontal networks on the topic of preparing programmes for the next period. We are preparing an analysis of the needs and wishes of members for education, on the basis of which we will prepare several different workshops and seminars, which we also plan to offer to non-members.

Throughout the year we actively participated in the **QU4LITY** project under the scope of H2020 initiative, which is expected to demonstrate, in a realistic, measurable, and replicable way, an open, certifiable and highly standardised, SME-friendly and transformative shared data-driven ZDM (Zero Defects Manufacturing) product and service model for Factory 4.0. In the scope of the project the SRIP FoF is working with the JSI Department for the Automation, Biocybernetics and Robotics as one of the leading partners in Work Package 8 and is collaborating with a consortium of partners to design and implement a virtualized platform that will consist of the project marketplace, where all the ZDM equipment will be listed and marketed, and the 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 2021.

In December 2018 we joined the Interreg Mediterranean project Panoramed as co-leader in the field of innovation. In 2020 we continued with work on our planned working commitments. We prepared the material for our short 2-months communication campaign in co-operation with the head of department for innovation and communications office. Together with our leading partner we concluded preparations for "ToR", one of the key documents, which was the basis of our tender for strategic projects in the field of innovation. In this period two particular projects were chosen via an open call. 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 the innovation policies in corelation with the transnational governance programmes of the Mediterranean region. Project B-Blue however acts on connecting communities of the Mediterranean. They are bringing together the key figures from the blue bio-technologies with the goal of increasing their capacities and coordination as a 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.

We participated at all the project meetings with presentations of our past work and plans for our future activities, which in times of the pandemic all took place online. Together with the lead partner, we also prepared a "Policy

Paper" document, which summarizes the key guidelines for innovation policy makers in the Mediterranean. We started with the preparation of "follow-up" strategic projects, which will be fully prepared in the first part of 2021. Within the Slovenian government (SVRK) we were also invited to participate in the working group for the preparation of a strategy for Interreg Mediteran. We started with the preparations for the "follow-up" of the strategic projects, which will be ready in the first part of 2021.

At the beginning of 2020, CToP started the implementation of 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 under 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 digitalisation and Industry 4.0. The project is based on a model called Value Hill, i.e., on the three pillars of the circular economy 1. model of circular product design 2. model of optimal use and 3. model of value restoration.

In 2020, three pillar-based expert working groups also involved JSI researchers from the Environment (O2) and Systems and Controls (E2) sections to help partners identify key challenges in the transition from a linear to a circular economy, and in particular support instruments making informed decisions for investments in digitalization and a change of business systems by companies that will have to adapt to the new European regulations in the field of plastics, water resources, waste and chemicals, recycling electronic devices and ICT waste, the use of digital data and other directives that are being adopted at the European Community level and will accelerate the transition to a green and more resilient economy.

In 2020 the so-called mapping of stakeholders operating in the Alpine region in the field of the circular economy in the public, research and economic sectors. A comparative study of good examples and practices of implementing circular systems using digitization and support tools was conducted for 26 regions in 8 countries among 15 project partners. Examples of good practice are from the automotive, furniture, food, health and bio-economics, packaging, textile, digital/electronics, education and consulting, and waste processing industries. A more detailed review of stakeholder needs within an individual circular economy model (product design, optimal use and restoration of value) was performed on individual segments of industrial production, which are strategically important areas in each of the participating regions, e.g., use of plastics in various industries, construction, textiles, food, wood and wood processing as a building material. As part of the product design group, which includes CToP, phases in the circular system were identified, e.g., in construction, material acquisition, construction, use of the building and end of the life cycle of the building; in industrial production the entire production-supply chain.

The strategies of the participating regions in implementing circular-economy systems were collected, including a review of enabling technologies and regional instruments to support the circular economy through digitalization, in the areas of environmentally friendly products, energy storage and distribution, energy efficiency, sustainable mobility, collection, sorting and waste recovery, recycling and sustainable management of water and other resources. As part of the second work package aimed at establishing circularity and digitality assessment tools and a training programme for companies and support organizations, CTop, with the active participation of two JSI research departments and an external contractor, prepared a training programme for faster transitioning to a circular economy for the entire Alpine region. Existing tools for assessing the circularity and assessing the degree of digitalisation of companies and, with the help of SRIP ToP members, also testing the usability of the proposed tools. These will enable companies a systematic and, above all, an informed and strategic way of judging what changes the company can implement and how much financial and other investments are needed for the company to move from a linear business system to a circular business system, including the transition to a new business model into a service-oriented company. Such a system of education and application of tools for circularity and digital assessment enables support organizations that advise start-ups, and especially company management, to make informed, strategic decisions for upgrading production systems, digitize and optimize business processes, make a different perception on waste as a resource and a different approach to product design, organizing and optimizing production systems and other business processes, ultimately leading to a carbon-neutral economy for the Alpine region using i4.0 technologies (robots, sensors, 3D prints, automation, AI, digital twins and other green economy applications such as for example new materials replacing raw materials or application of KETs such as plasma, photonics and many others).

A free training programme for intermediary organizations and companies, developed in collaboration with project partners by JSI, CTop and external contractors, will be available online in digital form for support organizations and companies and will be launched in all regions in 2021. A programme and tools for assessing circularity and digital maturity, developed within the project and/or selected from existing tools, are also the basis for the preparation of supporting financial and other instruments and assistance for more strategic and targeted planning of investments in companies, economic policies and instruments for accelerating the circular economies of regions, countries, financial, regulatory, research and other institutions interests with accelerating the transition to a green and digital economy in the coming years. The results of the project will be considered in the framework of the Alpine Region Action Plan for the Transition to a Circular Economy and more broadly within the European Union.

The project started on 1st October 2019 and ends in June 2022. The total value of the project is €2,560,692. Fifteen project partners cooperate from five Alpine countries - Austria, Italy, France, Slovenia, Germany: Amt der Salzburger Landesregirung, Associazione Fabbrica intelligente Lombardia, Austria Wirtschaftsservice Gesellschaft, Auvergne-Rhône-Alpes Enterprises, Bundesministerium Wur Digitalcha BWCON, Chamber of Commerce and Industry and Agriculture of Venice Rovigo, Chamber of Commerce and Industry of Var.

More information about Circular 4.0 project:
https://www.alpine-space.eu/projects/circular4_0/en/home
https://www.linkedin.com/company/circular4-0/about/

In the scope of the **HIA (High Impact Action)** project, financed by EC, SRIP FoF has in cooperation with the Slovenian Tool and Die Development Centre TECOS prepared and carried out three open calls: call for international experts, call for service providers and call for SMEs. Through these calls five Slovenian voucher-winning SME projects will be selected by the neutral committee in the form of an international expert group, which will be able to spend the funds for services from eligible service providers in order to upgrade their existing production cells so they are modular, reconfigurable, interconnected and demonstrate the ability to connect into a common manufacturing platform.

In the first phase of the project SRIP FoF has exploited the Slovenian knowledge within its partnership and with the help of external experts in the field of Industry 4.0, prepared specifications for the forementioned open calls. After the end of the projects, HIA looks to draw lessons from the production cell upgrade projects and prepare specifications, which would represent the basis on which a national demonstration centre could be build, where a practical approach towards a factory of the future would be demonstrated by a cumulation of Slovenian expertise.

INTERNATIONAL PROJECT

1. H2020 - QU4LITY; Digital Reality in Zero Defect Manufacturing
   Rudi Panjtar, B. Sc.
   European Commission

R&D GRANTS AND CONTRACTS

1. MED Governance Platform
   Rudi Panjtar, B. Sc.
   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
   Rudi Panjtar, B. Sc.
   Government Office of the Land of Salzburg
3. Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF)
   Rudi Panjtar, B. Sc.
   Ministry of Economic Development and Technology
4. Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF)
   Rudi Panjtar, B. Sc.
   Ministry of Economic Development and Technology

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