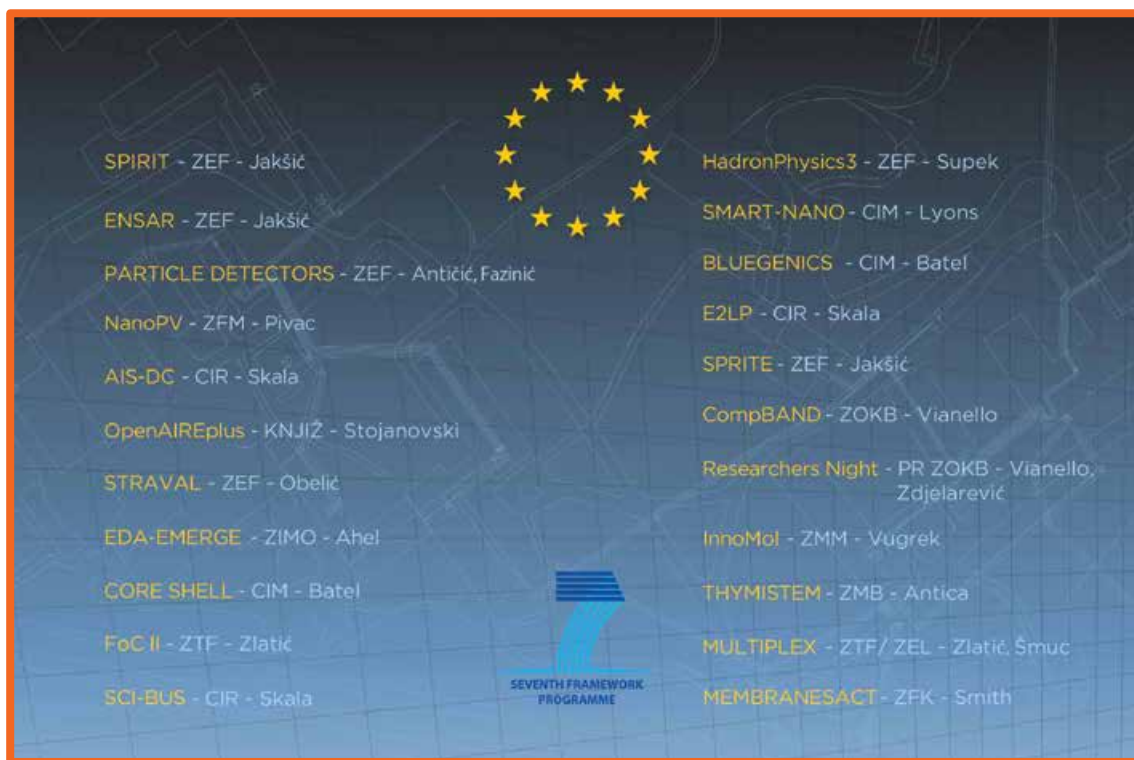


Ruđer Bošković Institute
Annual Report 2013

Ruđer Bošković Institute

Annual Report 2013



Zagreb, 2014.

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Dear reader,

The year 2013 was, in many ways, a remarkable year for the Ruđer Bošković Institute (RBI). Facing very significant budget cuts due to the ongoing economic crisis in Croatia, the RBI not only managed to continue its scientific excellence but, in fact, contracted a record amount through competitive international projects. The performance in terms of competitive domestic projects and, in particular, contracts with industry was also increased in 2013. Taking a more long term view, RBI continued the large-scale effort related to its flagship EU structural project, “Open Scientific Infrastructural Platforms for innovative applications in the economy and society (O-ZIP)”, valued in excess of 50 million EUR. This project is set to provide a major infrastructural investment at RBI and truly represents a game changer for Croatian science, innovation and technology.

Details of these and many more activities are to be found in the 2013 Annual Report of RBI. As the Director of RBI, I would like to sincerely thank the Editorial Board for preparing this report. I would also like to thank and congratulate the RBI scientists for making such a successful year possible.

Tome Anticic

Introduction

RBI OVERVIEW

The primary task of the Ruđer Bošković Institute (RBI) is to conduct excellent basic research, which is a prerequisite for the fulfilment of the other tasks that the RBI assumes in the development of the Republic of Croatia. These include the development of innovative research, participation in higher education, the transfer of knowledge to industry with the goal of developing new high-tech products and increasing public awareness of the importance and necessity of knowledge and science in modern society. The RBI carries out these tasks in collaboration with universities, scientific institutions and other related institutions in Croatia and abroad. The Institute is also strongly engaged in the promotion and popularization of science through numerous activities, such as, for example, a series of popular science lectures for the general public, which have become traditional fixtures at the Institute.

The RBI is regarded as Croatia's leading scientific institute in the natural and biomedical sciences as well as marine and environmental research, owing to its size, scientific productivity, international reputation in research, and the quality of its scientific personnel and research facilities. Moreover, the RBI is the leading and internationally most competitive Croatian institute by virtue of its participation in international research projects, such as the IAEA and EC FP5-7 programs funded by the European Commission, NATO, NSF, UKF, SNSF, DAAD and other international scientific foundations.

There are nearly 900 persons employed at the Institute today. Over 500 of them are scientists and researchers that pursue re-

search in more than 80 laboratories in theoretical and experimental physics, material physics and chemistry, electronics, physical chemistry, organic chemistry and biochemistry, molecular biology and medicine, marine science and the environment, information and computer sciences, laser and nuclear research and development.

Due to its manpower and well-organized infrastructure, including a large number of valuable experimental instruments, which comprise 50% of all scientific equipment in Croatia, the Institute is able to maintain its activities at the highest level.

The RBI aspires to contribute to the increasing competitiveness of Croatian economy and meeting the challenges of modern society through strengthened research and innovation capacity of RBI, while nourishing all three key priorities of the Horizon 2020 program: excellent science, industrial leadership and addressing societal challenges. RBI scientists are working to strengthen cooperation with industry. Thus, in recent years the number of research partnerships between industry and the RBI has a positive growth trend. This trend is largely conditioned by the participation of scientists RBI in European projects that foster cooperation with small and medium-sized enterprises.

Just a few weeks before Croatia's entry into the European Union on 1 July 2013, the RBI together with Brodarski Institute hosted the Annual Conference of the European Association of Research and Technology Organisations – EARTO, which was held in Dubrovnik. The conference, entitled "New Horizons For 2020 and Beyond: Croatia and South East Europe in the European Union", gathered about 250 of the EUs most successful representatives from the fields

of R&D, SME's and politics. This is the first time that Croatia has been provided with the opportunity to organise the EARTO Conference. This fact highlights the recognition of the RBI and Croatia as important partners in the European research and technology community and leading players in the promotion of scientific and technological research, economic development and innovation in the South-East European region.

RBI justified the confidence with excellent results regarding the EU and commercial projects. Since the beginning of FP7 programme implementation in 2007, RBI scientists have participated in 33 projects valued at around 11 million EUR. On this basis, RBI occupies the enviable position of the leading project-revenue generator in Croatia. Furthermore, in 2013 the RBI continued its strong collaboration with industry, both domestic and international such that the value of contracted contracts, as a proportion of total revenue, reached an all-time high.

In 2013, the RBI continued the large-scale effort related to its primary EU structural project, entitled "Open Scientific Infrastructural Platforms for innovative applications in the economy and society (O-ZIP)" and valued in excess of 50 million EUR. This project is set to provide a major and much-needed infrastructural investment in the RBI and truly represents a game changer for Croatian science, innovation and technology.

The main goal of O-ZIP is upgrading and unzipping of the RBI's intellectual property, capital equipment and know how, while increasing the RBI's impact in the ERA and boosting cooperation between scientific, academic and business sectors. By focusing on the RBI's most propulsive Key Enabling Technologies and reinforcing those parts of the RBI with the greatest commercial potential and proven excellence in providing European and applied projects, the project is designed to make a significant contribution to the creation of the basis for an innovation-based economy in Croatia. This will include the provision of a development platform for

start-up labs, SMEs and innovation incubators. By leveraging the existing capital equipment and investing in new, state-of-the-art infrastructure, the RBI will become one of the most competitive institutions in the region.

Apart from O-ZIP, the RBI has partnered with other institutions on three more structural projects, which have found their place on the indicative lists of the relevant ministries. These include: The Croatian Centre for Advanced Materials and Nano Technology (C2MAN, in partnership with the University of Zagreb and the Institute of Physics), The Croatian Scientific and Educational Cloud (HR-ZOO, in cooperation with the University of Zagreb Computing Centre), as well as the Science Educational Entertainment Centre (SEEC, in collaboration with the city of Zagreb).

Owing to its success on the EU level, the RBI is thus enabling targeted capital investment in infrastructure and equipment. Alongside with improving research quality through new projects and recruitments, the Institute thus enables the accessibility of excellent research, equipment and know-how already present at the RBI to the wider Croatian academic community and economic subjects. This strategy will contribute to a stronger integration of the RBI in the European Research Area (ERA) as a top scientific-research centre that strives to maximize the impact of its success on society as a whole.

ORGANIZATION OF THE RBI

Director General: Tome Antičić

Head of the Scientific Council: Miroslav Plohl

Chairman of the Board of Governors: Đuro Miljanić

International Scientific Board

Farooq Azam, University of California, USA
Fernando Azorin, Institute of Molecular Biology of Barcelona, Spain

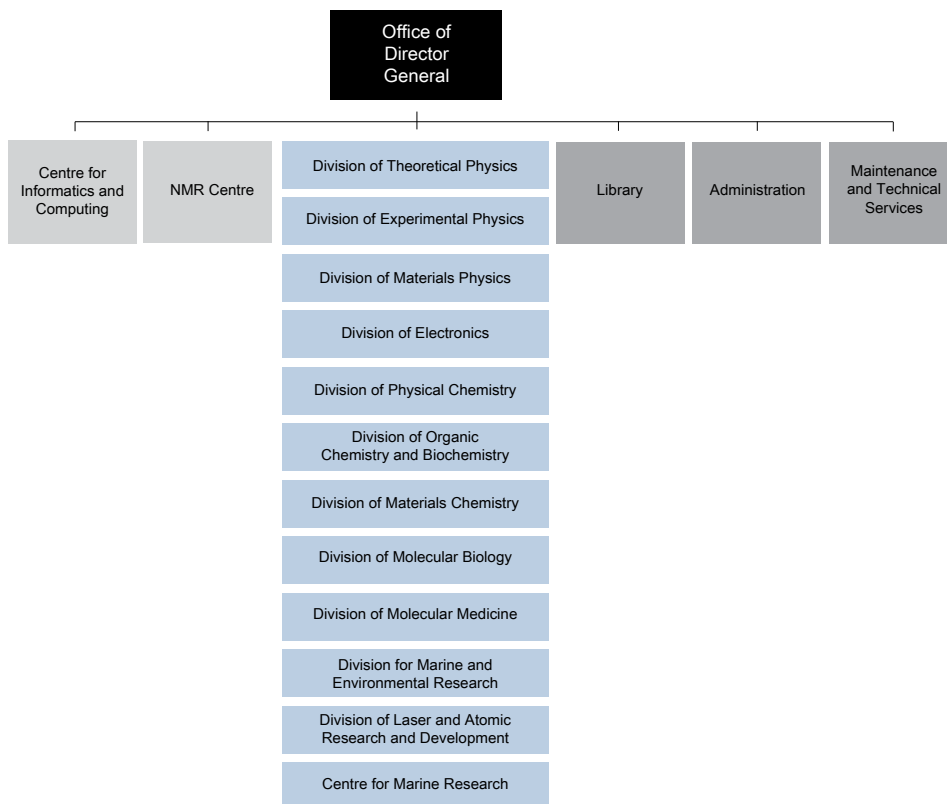


Figure 1. The organizational structure of the RBI.

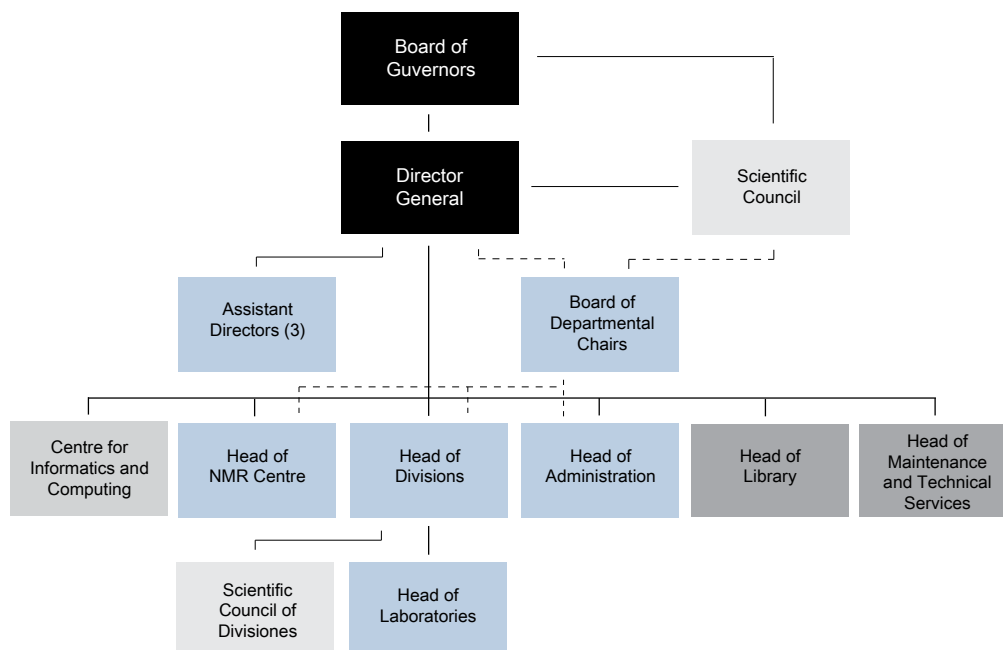


Figure 2. The administrative structure of the RBI

Jonathan R. Ellis, CERN, Switzerland
 Joshua Jortner, Tel Aviv University, Israel
 Bernd Kaina, Institut für Toxikologie,
 Germany
 Harold Kroto, University of Sussex, UK
 Jean-Marie Lehn, Institut de Science
 et d'Ingénierie Supramoléculaires,
 France
 Thomas C. Malone, University of Maryland
 Center for Environmental Science, USA
 Egon Matijević, Clarkson University, USA
 Jutta Ludwig Müller, Institute of Botany,
 Technische Universität Dresden,
 Germany
 Werner E.G. Müller, Johannes Gutenberg
 Universität, Germany
 Anthony R. Peaker, University of
 Manchester, UK
 Roberto D. Peccei, University of California
 Los Angeles, USA

Olivia Pereira-Smith, UT Health Science
 Center, USA
 Nadia Pinardi, University of Bologna, Italy
 Bogdan Povh, University of Heidelberg,
 Max-Planck-Institut für Kernphysik,
 Germany
 Miroslav Radman, Université René
 Descartes-Paris V, France
 Joseph Schlessinger, Yale University, USA
 Hans Joachim Seitz, Universität Hamburg,
 Germany
 Peter J. Stambrook, University of
 Cincinnati Medical Center, USA
 Rudolf Zechner, Institute for Molecular
 Biosciences, Austria
 Walter Giger, Swiss Federal Institute for
 Aquatic Sciences and Technology,
 Switzerland

2013	RESEARCH STAFF					TECHNICIAN S AND STAFF SCIENTISTS	ADMINISTRATI VE STAFF	MAINTAINANCE AND SECURITY	LIBRARY AND IT STAFF	TOTAL
	PERMANENT SCIENTISTS			POST- DOCTORAL FELLOWS	GRADUATE STUDENTS					
	Senior Scientists	Senior Research Associates	Research Associates							
Theoretical Physics Division	4	5	8	2	3	0	1	0	0	23
Division of Experimental Physics	12	10	10	9	13	9	1	1	0	65
Division of Materials Physics	5	6	8	1	7	2	1	0	0	30
Division of Laser and Atomic Research and Development	1	3	1	1	1	13	1	1	0	22
Division of Electronics	5	1	0	1	5	1	0	0	0	13
Division of Physical Chemistry	10	10	9	4	6	10	1	1	0	51
Division of Organic Chemistry and Biochemistry	8	11	16	15	12	12	1	3	0	78
Division of Materials Chemistry	6	7	18	7	4	12	1	1	0	56
Division of Molecular Biology	9	9	10	19	13	11	1	3	0	75
Division of Molecular Medicine	12	11	11	27	9	18	3	2	0	93
Division of Marine and Environmental Research	14	12	22	10	18	17	2	2	0	97
Centre for Marine Research	4	8	11	1	8	8	1	6	0	47
Centre for Informatics and Computing	1	0	2	0	3	0	0	0	6	12
Centre for Nuclear Magnetic Resonance	3	4	2	0	3	3	0	0	0	15
Library	0	0	0	0	0	0	0	0	10	10
Administration	0	1	0	0	1	7	50	26	0	85
Technical services	0	0	0	0	0	0	1	59	0	60
TOTAL	94	98	128	97	106	123	65	105	16	832

Table 1. Internal distribution of RBI employees

RBI LEADS IN RECEIVING EU FUNDS

By virtue of its performance the beginning of the FP7 programme, the RBI is the leading scientific institution in Croatia in terms of revenue generation from EU-projects. In 2013, the RBI was involved with some 100 active international projects (including 21 FP7, 2 IPA, 5 IAEA, 1 NATO, 37 COST, 2 SCOPES, and 45 bilateral projects), as well as around 50 domestic competitive projects and applied and technological contracts (including 7 HRZZ, 5 UKF, 1 HIT and 2 BICRO) and 129 projects in basic research funded by the Ministry of Science Education and Sport (see Table 2).

PROJECT	TOTAL NO.	FIELD OF RESEARCH
FP7	21	COMPUTER SCIENCES, EXPERIMENTAL PHYSICS, NANOMATERIALS, ENVIRONMENT
NATO	1	BIOMEDICINE AND MOLECULAR BIO SCIENCES
IAEA	5	EXPERIMENTAL PHYSICS
COST	37	BIOMEDICINE AND MOLECULAR BIO SCIENCES, NANO SCIENCES, CHEMISTRY, MOLECULAR SCIENCES AND TECHNOLOGY, ECOLOGY, FOOD AND AGRICULTURE, SOCIETY, CULTURE AND HEALTH
IPA	2	BIOMEDICINE, ENVIRONMENT
SCOPES	2	ENVIROMENT, EXPERIMENTAL PHYSICS

Table 2. A summary of international project success in 2013

Table 3 shows the actual revenues generated in 2013 by these projects and other sources of financing. Interested readers wishing to access a more detailed financial report are invited to contact the Institute. Already at the level of annual revenue, the growth in 2013 income from sources outside the domestic budget is apparent. Consideration of these extra-budgetary sources in terms of contracted yearly amounts, however, reveals an even more drastic improvement in this respect (Figure 3). This is particularly strongly manifested in the contracted international projects but the figures for competitive domestic projects and commercial activities also reflect a welcome positive trend in 2013. The commercial activities in 2013 results were primarily a result of numerous contracts with domestic companies, such as Podravka, HEP, Hrvatske vode, INA Croatia, Pliva and HS Produkt, and an ever growing number of such contracts with commercial entities in foreign countries.

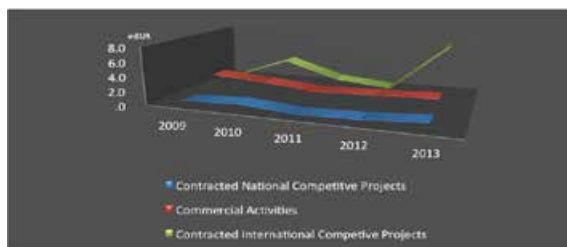


Figure 3. The trend in contracted project revenue since 2009

The largest FP7 infrastructure project with the highest budget in natural sciences ever

REVENUE (k€)	2008	%	2009	%	2010	%	2011	%	2012	%	2013	%
Funding from Ministry of Science, Education and Sports (MSES)	25.755,01	86,37%	24.030,18	83,82%	23.372,73	81,61%	21.628,32	87,40%	21.602,56	90,16%	20.486,04	76,99%
National project funding (Croatian Science Foundation, Croatian Institute of Technology, etc.)	487,60	1,64%	345,92	1,21%	1.365,29	4,77%	941,69	3,81%	452,73	1,89%	443,84	1,67%
International project funding (FP, NATO, IAEA, etc.)	910,31	3,05%	1.575,53	5,50%	1.780,55	6,22%	1.042,51	4,21%	526,51	2,20%	3.728,76	14,01%
Commercial contracts	2.449,66	8,22%	2.416,48	8,43%	1.873,09	6,54%	1.116,29	4,51%	1.372,34	5,73%	1.594,82	5,99%
Donations and other funding	216,62	0,73%	300,39	1,05%	246,15	0,86%	16,62	0,07%	6,22	0,03%	354,65	1,33%
TOTAL	29.819,20	100,00%	28.668,50	100,00%	28.637,81	100,00%	24.745,43	100,00%	23.960,36	100,00%	26.608,10	100,00%

Table 3. Actual revenue by source since 2008 (in Thousands of EUR).

to be conducted in Croatia was contracted by the RBI in 2013. The project, which was granted as part of the FP7-REGPOT grant scheme has a total value of 4.8 million EUR and is led by the Head of the RBI Division of Molecular Medicine, Oliver Vugrek. The project, entitled "Enhancement of the Innovation Potential in SEE through New Molecular Solutions in Research and Development (Inno-Mol)", will involve a team of almost 300 scientists from seven divisions of the RBI working together to establish an 'Innovation Pipeline'. The pipeline brings together the disciplines of Medicine, Biology, and Chemistry and aims to arrive at innovative new molecular solutions for the treatment and monitoring of numerous diseases, including cancer. The new human resources, capital equipment and networking opportunities provided by the project will be used to create a productive, state-of-the-art environment that is unique in the region and which will bridge the gap between the pre-commercial and commercial phases of R&D, thus enhancing the relevance of the RBI's position in the European Research Area (ERA).



Figure 4. The InnoMol team

The year of 2013 also saw the first award of a Starting Grant from the prestigious FP7-IDEAS scheme, coordinated by the European Research Council (ERC), to an RBI employee. The successful applicant was Ana-Sunčana Smith from the Division of Physical Chemistry, whose project "Biological Membranes in Action: A Unified Approach to Complexation, Scaffolding and Active Transport (MEMBRANESACT)" is valued at 1.5 million EUR over 5 years. In keeping with the

mission of the ERC, the project is concerned with fundamental research, which, in this case, is focussed on addressing intrinsically biological problems by means of theoretical physics. As such, the project will contribute to both physics and the life sciences by developing general principles that can be applied to processes in cells. An approach of this kind is of fundamental importance since it can identify how interactions on the cell surface arise and, therefore, may translate directly into pharmaceutical applications.

Mario Cindrić, from the Division of Molecular Medicine, was granted a project through the Instrument for Pre-Accession (IPA) for the development of a novel method of rapid detection of pathogens and tumour cells for use in clinical practice. The European Union has provided financial support for the project in the amount of approximately 530 000 EUR. The results of this research, which the RBI conducts in collaboration with the Faculty of Food Technology and Biotechnology of the University of Zagreb and SEMGEN Ltd., should contribute to future rapid clinical identification of pathogenic cells and biohazards by using the original method of biotypization while developing more effective diagnostics. This can be expected to lead to reduced and more selective use of antibiotics and more timely treatment of tumours. It is an innovative and marketable method used for the first time.

On the domestic front, RBI scientists continued their impressive record with the Unity through Knowledge fund in 2013. Of the 17 Cooperability projects awarded nationwide, 4 were coordinated by RBI scientists. In the Division of Molecular Medicine, Silva Katušić Hećimović's project "Lysosomal dysfunction as a common mechanism of neurodegenerative diseases" was valued at 230 000 EUR. Ivančica Bogdanović Radović, from the Division of Experimental Physics, was awarded a project in the amount of 140 000 EUR, entitled "Study of modern paint materials and their stability using MeV SIMS and other analytical techniques". The Division of Physical Chemistry, which houses Nađa Došlić, will

host her project "Time resolved photoelectron spectroscopy as a probe for ultrafast excited state dynamics", which is valued at 180 000 EUR. Igor Đerđ, of the Division of Materials Chemistry, will carry out a project under the title "Multifunctional complex metal tellurates: Structure-property relationship study" which carries a contracted value of 215 000 EUR. Finally, the project "Protein ADP-ribosylation in a model prokaryote *Streptomyces coelicolor* and human", worth 174 000 EUR, is to be co-led by Andrea Mikoč, from the Division of Molecular Biology. The project will be implemented in collaboration with the University of Oxford in the UK, where the project leader, Ivan Ahel, is currently employed.

CROATIA IS PARTICIPATING IN CREATING A "MINIATURE SUN"

The Croatian Fusion Research Unit (CRU), coordinated by the RBI, has joined the UK Fusion Association as an "External Research Unit" by signing a cooperation agreement in the Culham Centre for Fusion Energy, UK. This is of immense significance for the inclusion of Croatian scientists in research, development and application of thermonuclear fusion carried out by the European Union and the European Atomic Energy Community (EURATOM). Amongst other efforts, this also covers participation in the International Thermonuclear Experimental Reactor (ITER) project. ITER is the world's most advanced



Figure 5. RBI Director General Tome Antičić (far left) and CRU Coordinator Tonči Tadić (far right) at Culham Centre for Fusion Energy

experimental fusion reactor and is aimed at obtaining a more cost-effective, cleaner, safer and practically inexhaustible energy source. Valued at 13 billion EUR, this most significant scientific experiment of our times, will develop with the participation of the EU, USA, China, Russia, India, Japan and Korea, with the EU covering one half of all costs.

PAPERS PUBLISHED IN PRESTIGIOUS INTERNATIONAL JOURNALS

In 2013 RBI scientists published 681 research articles. Among these, 588 articles were published in journals indexed in WoS, the majority of which were published in high ranking international Journals.



Figure 6. Selected cover art featuring RBI publications.

Researchers from Division of Theoretical Physics Predrag Lazic and Damir Šokčević in collaboration with scientists from the Institute of Physics in Zagreb, the University of Cologne, the Research Centre in Jülich (Germany), and colleagues at the Brookhaven National Lab (USA) - published an article in the prestigious journal *Nature Communications* (IF = 10.015). The article, entitled "The mechanism of cesium intercalation of graphene" deals with the intercalated cesium per epitaxial graphene monolayer on the surface of iridium. This group of researchers parallel to this paper were also performed studies of intercalation of europium atoms which was published soon afterwards in the journal *Nano Letters*.

DEPARTMENT	STAFF	ARTICLES*						THESES			
		Articles in journals indexed in WoSCC***	Articles in other journals and chapters in books	Articles in conference proceedings	Total articles	Books	Patents	Theses (mentored by RBI staff)			
	Research staff**							Doctoral Theses (written by RBI staff)	Doctoral	Masters	Total mentored theses
Division of Theoretical Physics	22	21			21			1	1	3	4
Division of Experimental Physics	54	200	6	8	214	1		3	3		3
Division of Materials Physics	27	33	4	1	38				1	2	3
Division of Electronics	12	7	4	3	14						
Division of Physical Chemistry	39	54	2	2	58			1	3		3
Division of Organic Chemistry and Biochemistry	62	54	3	1	58			6	9	6	15
Division of Materials Chemistry	42	52	12	6	70			1	2	3	5
Division of Molecular Biology	60	39	7		46			5	6	9	15
Division of Molecular Medicine	70	59	10		69		1	4	6	7	13
Center for Marine Research	32	15		5	20			1	1	1	2
Division for Marine and Environmental Research	76	88	9	3	100			3	2	5	7
Division of Laser and Atomic Research and Development	7	6		1	7			1	1		1
NMR Centre	12	18	2	4	24					1	1
Centre for Informatics and Computing	6	10		3	13						
Library	0	2	3		5						
TOTAL	521	588	59	34	681	1	1	26	34	37	71

* Original scientific papers and review papers in journals/conference proceedings and chapters in books

** Scientists, post-doctoral fellows and graduate students

*** Articles published in journals and indexed in the following Web of Science Core Collection's (WoSCC) citation indexes - Science Citation Index - Expanded (SCI-Exp) and Social Science Citation Index (SSCI).

Table 4. Review of publications for the year 2013

Mario Vazdar, a research associate in the Division of Organic Chemistry and Biochemistry, in collaboration with colleagues from the Institute of Physical Chemistry in Prague, published a study which was selected to appear on the cover of the international journal *Faraday Discussions*. In their paper, entitled "Interactions of monovalent salts with cationic lipid bilayers", Vazdar and colleagues with the help of advanced software and ex-

perimental methods have shown that certain ions may increase or decrease the mobility of positively charged membranes, which are used in various medical purposes such as the development of gene therapy.

Krunoslav Užarević, a scientist of the Division of Physical Chemistry, in collaboration with his colleague Ivan Halasz and scientists from the Faculty of Science in Zagreb published a paper entitled "Dynamic Molecular

Recognition in Solid State for Separating Mixtures of Isomeric Dicarboxylic Acids" in one of the most influential journals in the field of chemistry, *Angewandte Chemie International Edition* (IF 13.455). The same journal also published a paper by Katarina Vazdar from the Division of Physical Chemistry, and her colleagues from the Institute of Organic Chemistry and Biochemistry at the Academy of Sciences of the Czech Republic and University of Tartu in Estonia. This paper, which was entitled "Very Strong Organosuperbases Formed by Combining Imidazole and Guanine Bases: Synthesis, Structure, and Basicity", investigates the preparation of new and very strong organic superbases, which do not contain toxic elements.

RBI physicists Saša Ceci, Milorad Korolija and Branimir Zauner published a research paper entitled "Model-Independent Extraction of the Pole and Breit-Wigner Resonance Parameters" in the prestigious journal *Physical Review Letters* (IF = 7.943). In this paper, the three authors proposed a new model independent method for determining the properties of short-lived subatomic particles directly from the experimental data.

Goran Štefanić, Stjepko Krehula and Ivka Štefanić from the Division of Materials Chemistry, published a paper in the prestigious scientific journal *Chemical Communications* (IF = 6.378). In the article entitled "The high impact of milling atmosphere on the steel contamination" the RBI scientists provided the first clear insight into the mechanism of interaction of the ground sample and steel balls (grinding tool) in standard high-energy milling in more and less oxidative atmospheres.

Further details of the many important discoveries made by RBI scientists in 2013 are to be found in the subsequent sections of this report.

INTERNATIONAL CONFERENCES AND POPULARIZATION ACTIVITIES

In 2013 RBI continued to support the organization of numerous international and domestic conferences which are mentioned in the subsequent sections of this report. At the same time, a concerted effort was made to significantly increase activities connected with the popularization of science. Some examples of these efforts are outlined below.

RBI was a partner of "The Researchers' Night" FP7 project. This pan-European event involves a wide range of scientific and research organisations, including museums, laboratories and academic institutions, which host a variety of entertaining and fun events planned to run late into the night. The aim is to give the public and, in particular, young people, the opportunity to meet researchers within the context of festive and 'fun' activities and to highlight the appeal of pursuing a research career. The Researchers' Night in Croatia took place in the three largest Croatian cities: Zagreb, Split and Rijeka. In Zagreb, the Ruđer Bošković Institute joined forces with the Agency for Mobility and EU Programmes as the project co-ordinator. Along with the Agency, the partner co-organizers were some of the largest research institutions in Croatia: University of Split, University of Rijeka, and



Figure 7. Researchers Night



Figure 8. RBI's Open Days

University of Zagreb, the Institute of Physics Zagreb, and Society science.org. In Croatia the event took place under the slogan Night of the Lab Out – NLO 2013, and that was exactly what we strove to achieve through our activities – to bring labs and their researchers, in as large a number as we could, to the streets and squares of Croatian cities.

Pursuing this idea, we located our activities in Zagreb at 4 venues at one of the Zagreb's main squares (popularly known as "Flower Square"), which has always been a prime meeting and strolling venue in Zagreb. The visitors were able to enjoy non-stop performances from 5 p.m. until 11 p.m. More than a hundred of scientists challenged the spectators' senses, perception, curiosity and knowledge through workshops, experiments, demos, a marathon of science shows, films, installations, research cafes, games and lots of surprises for all ages and all tastes. The project attracted more than 5 000 visitors in Zagreb involved more than 30 scientists from the RBI.

RBI also organized a large-scale pop-science event under the heading "RBI's Open Days". This three day event attracted more than a 4500 visitors, mainly children, which enjoyed in imaginative, creative, scientific adrenaline adventure compiled of a numerous scientific experiment demonstrations and interactive lectures, during which they were informed about crystals, atoms, bacteria, took a trip up to 50 000 years, discovered the invisible world of nanoparticles, walked through the valley of atomic nuclei and found out why chemistry is cute. This event was aimed to

demonstrate that science can be exciting, creative and playful, and that being a scientist means exploring the limitless possibilities. A special guest at the Open days was Nobel Prize laureate professor Dan Shechtman.

In addition to the high-profile events, RBI was involved with around 300 popularization-activities: lectures, scientific demonstrations, workshops for kids, etc. After launching the RBI Social media project focused on viral communication, the RBI Public Relations office continued extensive and dynamic communication successfully targeting different target demographics. Namely, active use of Face Book was targeted more towards the general public and less so towards the scientific and academic community. On the other hand, the official RBI LinkedIn profile was focussed more towards the needs of the business, scientific and academic sectors. The average public engagement rate on Facebook for each of the topics and posts released was indicative of the success of these efforts, breaking its record during the 2013 RBI Open days, reaching over 203 173 followers. This corresponds to 15 629 followers daily on the RBI Face Book profile. The Open Days event page saw a total of 69 013 followers, amounting to 5 308 users daily.

AWARDS AND RECOGNITION

The achievements of RBI scientists in 2013 were also recognized through numerous awards.

In the largest national competition for the best website in Croatia and the Region the results of the "VIDI WEB TOP 100 2012" were released in 2013. The RBI's website was recognized as one of the winners for 2012 and one of the best sites in the category "Government organizations, public institutions and public services".

In 2013, the Croatian Academy of Sciences and Arts awarded Nela Pivac, Laboratory of Molecular Neuropsychiatry, Division of Molecular Medicine for the highest achieve-



Figure 9. Helena Bilandžija and Željka Fiket at For Women in Science in 2013

ments in the field of medical science for the year 2012 for her scientific discoveries that represent contributions to understanding the molecular basis and treatment of neuropsychiatric disorders and behavioural disorders such as suicidal behaviour. DSc Pivac has so far published a total of 115 scientific papers in international journals which have been cited on more than 1 000 occasions as well as 24 book chapters. Her scientific research was included in two international databases - The Genetic Association Database (GAD) and Published International Literature on Traumatic Stress (PILOTS), which shows contribution to understanding the genetic basis of disease.

This annual award for the popularization and promotion of science in the field of natural sciences was awarded to Slobodan Bosanac of the Division of Physical Chemistry. Since 1986, Dsc Bosanac has been a key organizer of the Brijuni conference, which takes place every second year on the island of Brijuni and brings together leading international and Croatian scientists to discuss actual themes from a multidisciplinary perspective. Dsc Bosanac is also the president of the Croatian Astronomical Society and recently founded a branch of education worldwide network of Global Educational Outreach for Science, Engineering and Technology (GEOSSET) for Croatia based at the RBI. He has organized a number of popular science lectures, panel discussions and a variety of



Figure 10. Nela Pivac at the Croatian Academy of Sciences and Arts awards

events, including the "year of Astronomy" in 2009, as well as numerous successfully organized astronomical observations of the night sky, even in urban centers, which always gathered thousands of visitors and attracted wide media attention.

Vjekoslav Štrukil, from the Laboratory of Physical Organic Chemistry in the Division of Organic Chemistry and Biochemistry, was awarded the annual award for young scientists in the natural sciences. The prize was awarded for his scientific achievements in the field of guanidine chemistry and applications of the mehanochemical method for the synthesis of organic and organometallic compounds without the use of toxic organic solvents.

Gordana Nedic Erjavec, from the Laboratory for Molecular Neuropsychiatry in the Division of Molecular Medicine, was awarded the annual award for young scientists in the field of biomedical sciences. The award was based on her important contribution to field of biomedicine and health (neurosciences), as evidenced through her coauthorship of 24 scientific papers, on seven of which she is a main author, and her contributions to studies of the biological underpinnings of neuropsychiatric disorders.

Young RBI scientists Helena Bilandžija, from the Division of Molecular Biology, and Željka Fiket, from the Division for Marine and Environmental Research, received fellowships for national scholarship program "For

Women in Science" in 2013. For the seventh year in a row, the fellowships were awarded by the Croatian Commission for UNESCO, the Ministry of Culture and company L'Oreal Adria as a recognition of young scientists for their contribution to the development of science in Croatia, but also as a stimulus for further work primarily on their doctoral dissertations and for research work in institutions in Croatia and abroad.

The humanitarian action "Terry Fox Run" donated almost 10 000 EUR to the RBI Laboratory for Hereditary Cancer. The funds will be used for research of molecular mechanisms that are activated in response to the process of tumour cells to chemotherapy and for the procurement of equipment and chemicals necessary for the implementation of comprehensive and high-quality cancer research in the laboratory.

In 2013, the RBI also joined the European Committee for Marine Research (European Marine Board - EMB) – a unique strategic European Organization for research and the ocean, and the development of new technologies. Membership in the EMB will allow the RBI to remain completely up to date with the latest trends in the field of marine science and to participate in the creation of European policies related to Marine and Coastal Research and the development of new technologies.

EDUCATION

Although the RBI does not have the legal possibility of independently conducting doctoral studies, it has initiated a large number of doctoral and specialist studies in cooperation

	Academic year					
	2008/09	2009/10	2010/11	2011/12	2012/13	2013/14
Number of undergraduate courses	315	378	373	382	403	415
Number of graduate courses	166	179	174	174	179	181
Number of postgraduate (PhD) courses	33	48	40	42	41	44
Supervision of graduate theses	203	228	220	223	223	230
Number of specialist postgraduate programme courses	275	335	323	339	353	373
Organizing and holding professional program courses	157	172	168	170	174	178
Number of undergraduate courses	8	10	10	9	16	15
Number of graduate courses	384	459	617	523	723	764
Supervision of graduate theses	42	65	77	73	76	80
Supervision of postgraduate (PhD) programmes	37	53	53	58	58	62
Number of specialist postgraduate programme courses	198	216	198	208	213	214
Number of postgraduate (PhD) courses	3	4	4	6	7	7
Organizing and holding professional program courses	5	1	0	0	5	3
Participation of research assistants in teaching (number of courses)	4	5	4	3	4	3

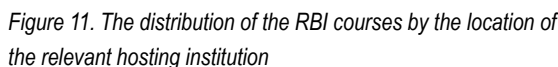
Table 5. Overview of the teaching activities of RBI staff from 2008-2013.

By far the strongest collaboration is with the University of Zagreb, with which a formal cooperation agreement was signed in 2007. Most of this cooperation takes place at the Faculties of Science, Electrical Engineering and Computing, Agriculture and Medicine. Together with the Josip Juraj Strossmayer University in Osijek, in 2002 the RBI launched the interdisciplinary postgraduate study Nature and Environmental Protection, which has operated as doctoral and specialist studies since 2008.

and RBI scientists teach a total of 72 courses in this program. The same year saw an agreement signed with the University of Rijeka for launching Undergraduate, Graduate and Doctoral studies in Medicinal Chemistry.

It should be particularly noted that during the recent past, research assistants of the Institute were included in teaching, especially in conducting practical and laboratory exercises and seminars. From 2008 to 2013, the number of courses per scientist was approximately 1.3, which indicates a high rate of participation by RBI scientists in university study programs. Details can be seen in Table 5 as well as Figures 11 and 12.

Apart from fundamental research and education, the activities of the RBI also result in various forms of intellectual creations. One important aspect of the RBI's mission is the protection of intellectual property and its commercialization. In this context, various specific activities have been initiated and realized over the last few years. As a subsidiary, the Ruđer Bošković Institute established Ruđer Innovations Ltd., a company specializing in the commercialization of innovations and technology transfer. The intellectual property portfolio of Ruđer Innovations includes innovations protected by patents or patent applications in various fields of sci-



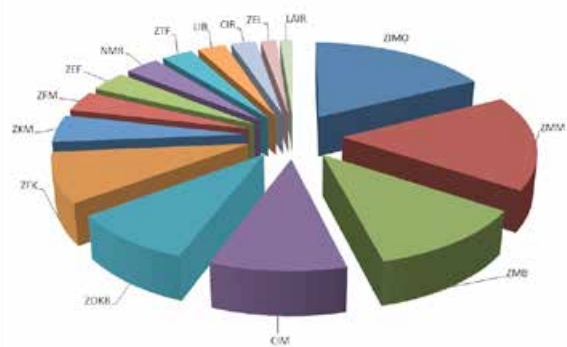


Figure 12. The distribution of the RBI courses by RBI Division

ence that have commercial potential. In 2013 RBI had one patent accepted and three patent applications:

US Patent 8,389,505 - ADAMANTANE DERIVATIVES OF AZA CROWN ETHERS

AND THEIR USE IN TREATMENT OF TUMOR was issued to M. Kralj, K. Majerski, T. Šumanovac Ramljak, M. Marjanović.

US Patent Office received application US 14/117,395 - METHOD OF DETECTION OF AMINO ACID SEQUENCE AND/OR IDENTIFICATION OF PEPTIDES AND PROTEIN, BY USE OF A NEW DERIVATIZATION REAGENT AND SYNTHESIS OF 5-FORMYL-BENZENE-1,3-DISULPHONIC ACID AS DERIVATIZATION REAGENT, by M. Cindric, Z. Hamersak, I. Dodig. The same patent was also applied to Canadian patent office CA 2,863,114.

US Patent Office received application US 61/917,371 - CHOLESTEROL ABSORPTION INHIBITORS, by I. Habuš i T. Dražić.

DIVISIONAL ORGANIZATION

Head: Željko Crljen

The Theoretical Physics Division (ZTF) consists of the following laboratories:

- ⇒ Solid State Physics Group, Damir Šokčević
- ⇒ Particle Physics and Cosmology Group, Blaženka Melić
- ⇒ Theoretical and Mathematical Physics Group, Stjepan Meljanac



OVERVIEW OF THE DIVISION

Research activities in the Theoretical Physics Division are focused on broad areas of theoretical physics, including particle physics, gravity, cosmology, mathematical physics, quantum field theory, condensed matter physics and complex systems.

The particle physics and cosmology section of the Division does research in particle and collider physics and cosmology with investigations on perturbative quantum chromodynamics, heavy hadrons, astroparticle cosmology, dark matter and dark energy, and matrix models and duality. Research on quantum field theory and symmetry on non-commutative spaces and integrable systems are a core interest of the theoretical and mathematical physics section. Research in condensed matter physics focuses on the electronic and magnetic properties of nanoscale systems including spin and charge transport of hybrid nanostructures, graphene and re-

lated systems, the statistical physics of non-equilibrium phenomena and the dynamical complex systems.

The Division has a strong commitment to excellence in research and international scientific exchange and collaboration. Members of the Division are engaged in a multitude of activities reaching far beyond the boundaries of the division through international bilateral collaborations and projects, organizing of conferences, as well as involvement in lecturing at the universities of Zagreb and Split.

TOP ACHIEVEMENTS

Interface-engineered templates for molecular spin memory devices

Recently, the use of molecular spin state as a quantum of information for storage, sensing and computing has generated considerable interest. A molecular device was constructed using phenalenyl moieties, which can be regarded as graphene fragments, to engineer interfacial spin transfer

resulting from the hybridization and magnetic exchange interaction of phenalenyl with the surface of a ferromagnet and having an unexpected interfacial magnetoresistance of more than 20 per cent near room temperature (Raman et al., 2013).

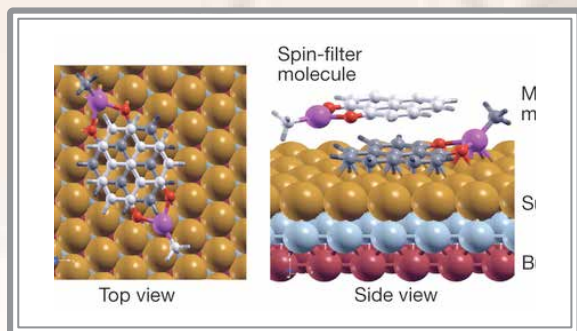


Fig. 1. Interface model for DFT calculations: top view (left) and side view (right) of the relaxed molecules' configuration on a Co(111) surface; grey, carbon; red, oxygen; purple, zinc.

The backside of graphene: manipulating adsorption by intercalation

By partial intercalation of graphene on Ir(111) with Eu or Cs we induce strongly n-doped graphene patches through contact with these intercalants. They coexist with nonintercalated, slightly p-doped graphene patches. We employ these backside doping patterns to directly visualize doping induced binding energy differences of ionic adsorbates to graphene through low-temperature scanning tunneling microscopy. Density functional theory confirms these binding energy differences and shows that they are related to the graphene doping level (Schumacher et al., 2013).

The mechanism of caesium intercalation of graphene

The microscopic mechanisms and dynamics of graphene intercalation are not well understood. We find that the intercalation of alkali atoms under epitaxial graphene is adjusted by the van der Waals interaction, with the dynamics governed by defects anchored

to graphene wrinkles. Our findings are relevant for the future design and application of graphene-based nano-structures (Petrović et al., 2013).

Matrix theory origins of non-geometric fluxes

We explored the origins of non-geometric fluxes within the context of M theory described as a matrix model. Building upon compactifications of Matrix theory on non-commutative tori and twisted tori, we formulate the conditions which describe compactifications with non-geometric fluxes. These turn out to be related to certain deformations of tori with non-commutative and non-associative structures on their phase space. Quantization of flux appears as a natural consequence of the framework and leads to the resolution of non-associativity at the level of the unitary operators. The quantum-mechanical nature of the model bestows an important role for the phase space. In particular, the geometric and non-geometric fluxes exchange their properties when going from position space to momentum space thus providing a duality among the two. Moreover, the operations which connect solutions with different fluxes are described and their relation to T-duality is discussed. Finally, we provide some insights on the effective gauge theories obtained from these matrix compactifications (Chatzistavrakidis and Jonke, 2013).

Generalized models of unification of dark matter and dark energy

A model of unification of dark matter and dark energy based on the modeling of the speed of sound as a function of the parameter of the equation of state is introduced. It is found that the model in which the speed of sound depends on the power of the parameter of the equation of state contains the generalized Chaplygin gas models as its subclass. A constraint on model parame-

ters is obtained using observational data on the Hubble parameter at different redshifts (Čaplar and Štefančić, 2013).

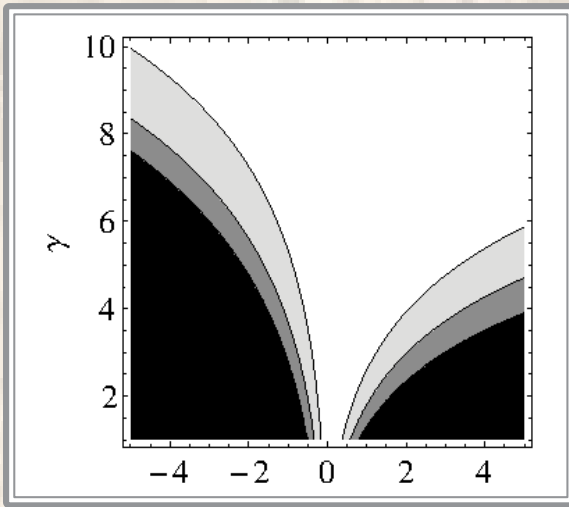
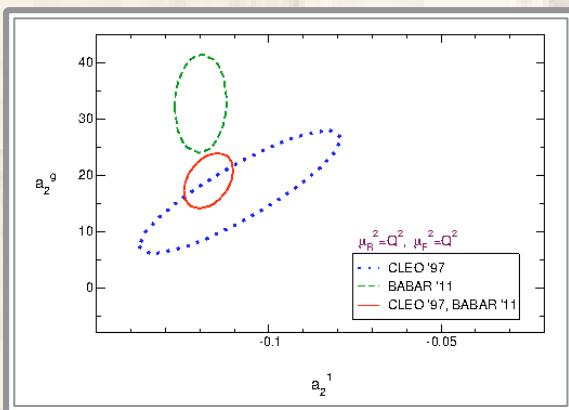


Fig. 2. The 68.3% (white), 95.4% (light gray) and 99.7% (gray) probability contours in the model parameter plane from the data on Hubble parameter at different redshifts and for the present Hubble parameter value $h = 0.702$.

The η (η') gamma transition form factor and the gluon–gluon distribution amplitude

The eta-gamma and eta'-gamma transition form factors are analyzed to leading-twist accuracy and next-to-leading order (NLO) of perturbative QCD. Using an



Correlation between eta distribution amplitude Gegenbauer coefficients a_{12} and a_{g2} (left) and their evolution (right). The 1σ χ^2 -contours are shown for fits to the data from only CLEO, BABAR and to both data sets (left). The shaded bands indicate the errors of the coefficients obtained using both data sets (right)

eta-eta' mixing scheme and all currently available experimental data the lowest Gegenbauer coefficients of the distribution amplitudes for the valence octet and singlet quark-antiquark and the gluon-gluon Fock components are extracted. Predictions for the $g^*g^*\eta'$ vertex function are presented. We also comment on the new BELLE results for the pi-gamma transition form factor (Kroll and Passek-Kumerički, 2013).

Different realizations of kappa-momentum space and relative-locality effect

Different realizations for the momentum sector of kappa-Poincare Hopf algebra, which is associated with a curved momentum space are analyzed. It is shown that the notion of the particle mass as introduced in the context of relative-locality is realization independent for a wide class of realizations. However, the time delay formula clearly shows a dependence on the choice of realization (Meljanac et al., 2013).

Differential forms and k-Minkowski spacetime from extended twist

The construction of κ -deformed coordinates and forms (super-Heisenberg algebra) using extended twist was presented. It was shown that it is compatible with the bicovariant differential calculus with κ -deformed $igl(4)$ -Hopf algebra. The extended twist leading to κ -Poincare-Hopf algebra was also discussed (Jurić et al., 2013).

K-Poincare-Hopf algebra and Hopf algebroid structure of phase space from twist

It was shown that the quantum phase space has a Hopf algebroid structure and that the application of the twist on it leads to a κ -deformed Hopf algebroid structure and κ -deformed phase space. Furthermore, κ -Poin-

care-Hopf algebra and κ -Minkowski spacetime are explicitly constructed from twist (Jurić et al., 2013).

EDUCATION

In 2013, the members of the Division continued to be involved in providing undergraduate and graduate courses mostly at the University of Zagreb (Faculty of Science, Faculty of Electrical Engineering and Computing), Zagreb School of Economics and Management and the University of Split (Faculty of Science) and the Catholic University of Croatia. They have supervised a number of B. Sc., M. Sc. and Ph. D. theses.

PROJECTS

Projects supported by the Ministry of Science, Education and Sport

1. Surfaces and nanostructures: Theoretical approaches and numerical calculations, Damir Šokčević
2. Electronic properties of hybrid nanostructures, Željko Crljen
3. Fundamental interactions in elementary particle physics and cosmology, Goran Duplanić
4. Quantum field theory, noncommutative spaces and symmetries, Stjepan Meljanac

Research, developmental and international project

1. Geometry and quantum field from noncommutative landscape, Larisa Jonke (Croatian-Austrian bilateral project), MSES, EUR 2.600
2. Forecasting Financial Crises, Vinko Zlatić (EU FP7-ICT-255987 – FOC-II Project), EUR 170.560
3. Foundational Research on MULTILEVEL COMPLEX networks and systems, Vinko Zlatić (EU-FP7-ICT-317532 – MULTIPLEX) from November 2013, EUR 263.652

SELECTED INVITED LECTURES

1. Lazić P, Materials genome – search for water splitting materials, 20th Croatian-Slovenian Annual meeting "Vacuum science and technique" Jerusalem, Slovenija, May 9-10, 2013.
2. Crljen Ž, Electronic properties of hybrid nanostructures, SYMONE Workshop, Dresden, Germany, May 30-31, 2013.
3. Štefančić H, Modified gravity and the relaxation of a large cosmological constant, 2nd Mediterranean Conference on Classical and Quantum Gravity (2nd MCCQG), Veli Lošinj, Croatia, June 9-15, 2013.
4. Melić B, Pionic dark matter, Workshop „Selected Challenges in Particle Phenomenology – Brda 2013“, Belica, Brda, Slovenia, September 18-20, 2013.
5. Crljen Ž, First principles modeling of the electronic structure and transport of nanoscale devices, Thermoelectrics 2013: New Thermoelectric Materials, Split, Croatia, September 28 – October 2, 2013.
6. Lazić P, Thermoelectrics – insights from first principles, Thermoelectrics 2013: New Thermoelectric Materials, Split, Croatia, September 28 – October 2, 2013.
7. Lazić P, Intercalation under epitaxial graphene, 8th Scientific Meeting of the Croatian Physical Society, Primošten, Croatia, October 6-8, 2013.
8. Melić B, Particle physics after Higgs discovery, 8th Scientific Meeting of the Croatian Physical Society, Primošten, Croatia, October 6-8, 2013.
9. Nesti F, Dark matter distribution in galaxies, Workshop on Future of Dark Matter Astrophysics: Insights and Perspectives, Trieste, Italy, October 8-11, 2013.
10. Nesti F, Galactic dark matter distribution, IX International Workshop - The "Dark Side of the Universe 2013", Trieste, Italy, October 14-17, 2013.

SELECTED ORGANIZED CONFERENCES

1. 20th Croatian-Slovenian Annual meeting "Vacuum science and technique", Jerusalem, Slovenia, May 9-10, 2013 (Damir Šokčević)
2. 2nd Mediterranean Conference on Classical and Quantum Gravity (2nd MCCQG), Veli Lošinj, Croatia, June 9-15, 2013 (Larisa Jonke)
3. 6th Austrian-Croatian-Hungarian Meeting-Summer Workshop for Theoretical Physics: "Nonabelian Gauge Theories and Quark Matter", Rab, Croatia, August 30 - September 4, 2013 (Kornelija Passek-Kumerički)
4. From Majorana to LHC: Workshop on the Origin of Neutrino Mass, Trieste, Italy, October 2-5, 2013 (Fabrizio Nesti)

SELECTED PUBLICATIONS

1. Raman K V, Kamerbeek A M, Mukherjee A, Atodiresei N, Sen T K, Lazić P, Caciuc V, Michel R, Stalke D, Mandal S K, Bluegel S, Muenzenberg M, Moodera J S. Interface-engineered templates for molecular spin memory devices. *Nature* **493** (2013) 509.
2. Schumacher S, Wehling T O, Lazić P, Runte S, Foerster D F, Busse C, Petrovic M, Kralj M, Bluegel S, Atodiresei N, Caciuc V, Michely T. The Backside of Graphene: Manipulating Adsorption by Intercalation. *Nano Lett* **13** (2013) 5013.
3. Petrović M, Šrut-Rakić, I, Runte S, Busse C, Sadowski J, Lazić P, Pletikosić I, Pan Z H,

- Milun M, Pervan P, Atodiresei N, Brako R, Šokčević D, Valla T, Michely T, Kralj M. The mechanism of caesium intercalation of graphene. *Nat Commun* **4** (2013) 2772.
4. Chatzistavrakidis A, Jonke L. Matrix theory origins of non-geometric fluxes. *J High Energy Phys* **02** (2013) 040.
5. Bilić N, Tolić D. Trapped surfaces in a hadronic fluid. *Phys Rev D* **87** (2013) 044033.
6. Bilić N, Tolić D. FRW universe in the laboratory. *Phys Rev D* **88** (2013) 105002.
7. Čaplar N, Štefančić H. Generalized models of unification of dark matter and dark energy. *Phys Rev D* **87** (2013) 023510.
8. Kroll P, Passek-Kumerički K. The H (H') gamma transition form factor and the gluon-gluon distribution amplitude. *J Phys G* **40** (2013) 075005.
9. Ma E, Melić B. Updated S3 model of quarks. *Phys Lett B* **725** (2013) 402.
10. Horvat R, Ilakovac A, Trampetić J, You J. Self-energies on deformed spacetimes. *J High Energy Phys* **1311** (2013) 071.
11. Meljanac S, Pachol A, Samsarov A, Gupta, Kumar S. Different realizations of kappa-momentum space. *Phys Rev D* **87** (2013) 125009.
12. Jurić T, Meljanac S, Štrajn R. Differential forms and κ -Minkowski spacetime from extended twist. *Eur Phys J C* **73** (2013) 2472.
13. Jurić T, Meljanac S, Štrajn R. K-Poincare-Hopf algebra and Hopf algebroid structure of phase space from twist. *Phys Lett A* **377** (2013) 2472.



DIVISIONAL ORGANIZATION

Head: Milko Jakšić

The Division of Experimental Physics consists of the following laboratories:

- ⇒ Laboratory for hadron physics, Ivan Supek
- ⇒ Laboratory for nuclear physics, Zoran Basrak
- ⇒ Laboratory for astroparticle physics, Raul Horvat
- ⇒ Laboratory for electromagnetic and weak interactions, Milica Krčmar
- ⇒ Laboratory for ion beam interactions, Milko Jakšić
- ⇒ Laboratory for measurement of low-level activities, Nada Horvatinčić
- ⇒ Laboratory for high energy physics, Krešo Kadija
- ⇒ Laboratory for nuclear analytical methods, Jasmina Obhodž
- ⇒ Group for hadronic spectroscopy, Alfred Švarc



radiation applications. The division staff is involved in international collaborations at experimental facilities abroad and in Croatia and maintains a strong involvement in both basic and applied physics research. A large fraction of the Division's financing comes from external sources and was mainly used to significantly enhance its experimental capabilities.

The main strategic objectives of the DEP are:

- A significantly enlarged experimental contribution to international physics collaborations, in particular by enhancing the contribution of local experimental work, leading to a much more prominent role in these experiments.
- Increased experimental capabilities and capacities for experiments at the local RBI Tandem accelerator facility. Increased utilization of other local experimental capabilities and in particular the Cockcroft Walton accelerator (neutron generator), laboratories for low level radiation measurements and detector testing capabilities using radiation sources and laser light.
- Exploration of application possibilities through interdisciplinary work such as modification and characterisation of ad-

OVERVIEW OF THE DIVISION

The core activities of the Division of Experimental Physics (DEP) involve experimental ion beam, nuclear, particle and astroparticle physics, as well as related

vanced materials using ion beams, C-14 dating using accelerator mass spectrometry, applications of PET isotope imaging capabilities in medicine, employment of radiation techniques in detection of explosives and interdisciplinary research related to fusion.

- Improved cooperation with universities by increasing the role of DEP resources in education both in terms of teaching and experimentation. Recruitment of the best doctoral and postdoctoral candidates as well as the funding sources for their education.
- Strengthened partnerships at numerous levels with prominent research institutions in Europe and internationally as a basis for increasing both research quality and external funding.

TOP ACHIEVEMENTS

CMS experiment at the LHC in CERN

The Compact Muon Solenoid (CMS) experiment at the Large Hadron Collider (LHC) has continued its exploration of the TeV scale and has produced many results, which resulted in a large number of publications in top journals. The detailed study of the newly discovered boson in 2012 at a mass of about 125 GeV has confirmed that the new particle has most of the expected properties of the Higgs boson as predicted in the Standard Model of elementary particles. The mechanism of mass generation through spontaneous symmetry breaking predicted by Higgs and others in the sixties can therefore be regarded as confirmed. This resulted in the 2013 Nobel prize in Physics being awarded to Peter Higgs and Francois Englert. The RBI group in the CMS Collaboration continued its active participation in the extraction of physics results from the LHC data and in the operation of the CMS detector. RBI scientists have in particular contributed to measurements of Standard Model processes and the search for New

Physics signals through studies of diboson final states. Their work resulted in some of the most stringent available limits on some New Physics scenarios. In the course of 2013, the RBI CMS group also increased its involvement in the operation and better understanding of the CMS Pixel detector, and developed several laboratory setups for pixel detectors at RBI, that will allow RBI to play an active role in future upgrades of the CMS pixel detector (Chatrchyan et al., 2013a; 2013b).

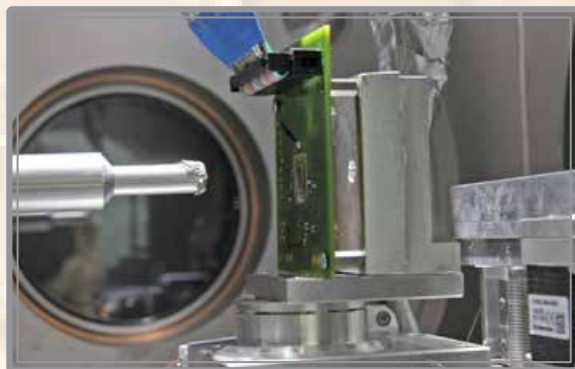


Fig. 1. Irradiation of CMS Pixel detector at the RBI Accelerator facility.

A unified description of fusion excitation function

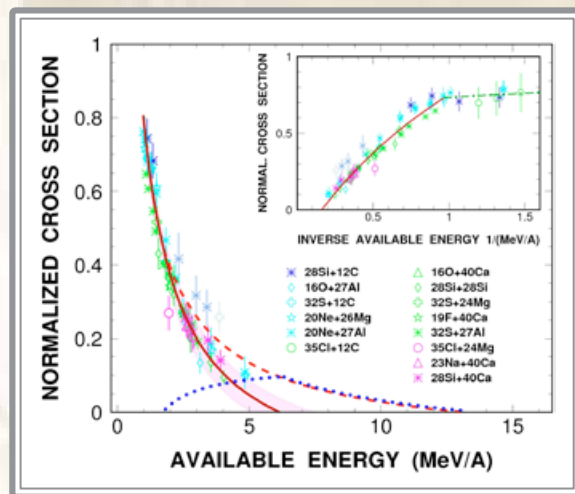


Fig. 2. Normalized and energy scaled complete fusion data and their best fit by a homographic function (full curve). Dashed curve is due to the same kind of fit to 238 complete+incomplete fusion data pertaining to 48 reaction systems while dotted one is difference of both and represents the incomplete fusion contribution. Inset shows a novel representation of fusion excitation function allowing to identify different regimes of fusion.

It has been shown that a properly scaled fusion excitation function complies with a universal homographic law, which is, within experimental errors, reaction system independent. From such complete and summed complete and incomplete fusion excitation functions we extracted the limiting energy for the complete fusion and the main characteristics (onset, maximum and vanishing) of the incomplete fusion (see figure). The DYWAN microscopic transport model correctly predicts the fusion cross-section and suggests that nuclear transparency is at the origin of fusion disappearance (Eudeset al., 2013).

Fusion barrier distributions from backscattering of the ${}^6\text{Li}$ on ${}^{64}\text{Zn}$

Measured excitation functions of quasi-elastic scattering of ${}^6\text{Li}$ and ${}^7\text{Li}$ projectiles on a ${}^{64}\text{Zn}$ target at backward angles around the Coulomb barrier allowed derivation of the corresponding barrier distributions (see figure3). The comparison between the data and coupled-channel predictions shows that the effects of channels not included in the calculations, such as direct breakup and transfers, are much larger for ${}^6\text{Li}$ than for ${}^7\text{Li}$ (Zadro et al., 2013).

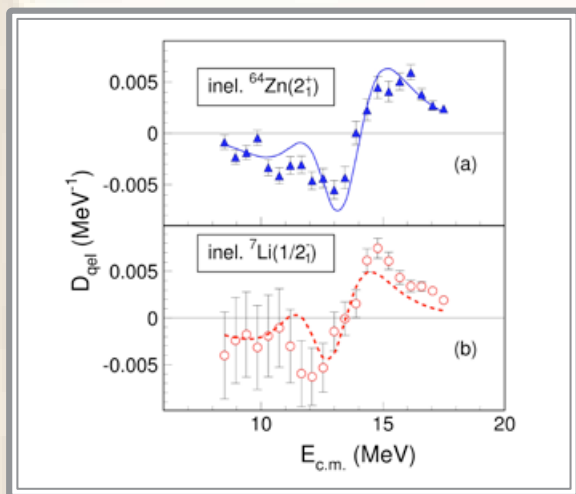


Fig. 3. Quasielastic barrier distributions of (a) inelastic ${}^{64}\text{Zn}(2_1^+)$ (filled triangles), and (b) inelastic ${}^7\text{Li}(1/2_1^+)$ (empty circles) derived from corresponding backscattering excitation functions for the ${}^7\text{Li} + {}^{64}\text{Zn}$ system. The curves are results of coupled-channel calculation.

Structure of neutron-rich chlorine isotopes

The Prisma magnetic spectrometer-Clara γ array setup has been used to investigate moderately neutron-rich chlorine isotopes populated in the ${}^{40}\text{Ar}+{}^{208}\text{Pb}$ multiple transfer reaction. Applying the particle- γ coincidence technique and combining new γ transitions identified in this measurement with previously available data allowed establishment of level schemes for the ${}^{37}\text{Cl}$ to ${}^{43}\text{Cl}$ isotopes. A favourable comparison of such level schemes with the results of large-scale sd - pf shell-model calculations allowed us to deduce by inspection the shell-model wave functions during the evolution of energy splitting between the $s_{1/2}$ and $d_{3/2}$ orbitals and the increased mixing of different proton configurations in the populated Cl isotopic chain (Szilner et al., 2013).

Search for dark matter particles

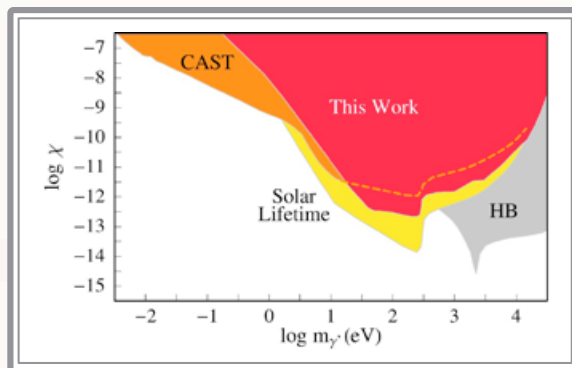


Fig. 4. Limits on the mixing parameter as a function of the hidden-photon mass from this experiment against the current hidden photon bounds.

In an experiment performed at the RBI (Laboratory for electromagnetic and weak interactions) we have searched for hidden photons coming from the Sun by observing the photoelectric-like process on germanium atoms inside the HPGe detector. Our constraints on the mixing parameter in the mass region from 20 eV up to 15 keV proved slightly better than those obtained recently by using data from the CAST experiment, albeit

still somewhat weaker than those obtained from solar and HB stars lifetime arguments (Horvat et al., 2013).

Ultra-thin diamond membrane detector

A unique transmission type single-ion detector based on diamond membrane has been constructed and tested at RBI in collaboration with JAEA Takasaki and CEA Saclay. An ultra thin diamond membrane simultaneously serves as a vacuum window and allows the extraction of an ion microbeam into the atmosphere. The negligible intrinsic-noise provides an excellent signal-to-noise ratio and enables a hit-detection efficiency of close to 100%, even for energetic protons, while the thinness of the membrane limits microbeam divergence (Grilj et al., 2013). This unique detector will open up new areas of single ion irradiation applications such as those using living cells.

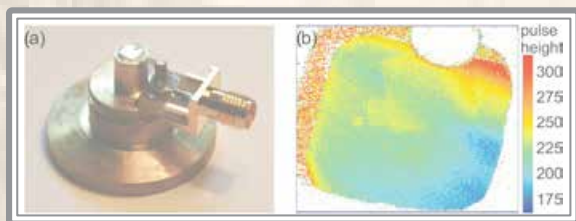


Fig. 5. Diamond membrane detector assembly (a) and IBIC image of charge collection distribution within the $1 \times 1 \text{ mm}^2$ area of the detector (b).

Collaboration TANGRA – Tagged Neutrons and Gamma RAYS

The LNAM group has been one of the world leaders in the use of tagged neutron techniques for various applications. The group was especially successful in development of tagged neutron techniques for field detection of hazardous substances such as explosives, drugs and toxic substances in cargo containers and in sunken objects on the sea floor. In 2013 the LNAM group was actively engaged in forming the TANGRA collaboration with several nuclear laborato-

ries including the Russian Joint Institute for Nuclear Research, Moscow State University, Moscow All-Russian Automation Research Institute and Bulgarian Institute for Nuclear Research and Nuclear Energy. The collaboration was formed with the aim to use and further develop tagged neutron techniques for fundamental and applied research. Applied research will include environmental applications, applications in the mining industry and applications in Martian soil survey. Fundamental research will include studies of rare nuclear processes induced by fast neutrons ($n, n'\gamma$), ($n, 2n'$), (n, n'). One of the experiments to be performed at the Ruder Boskovic Institute is shown in Figure 1. These processes are extremely important in studying the original patterns of nuclear synthesis during the Big Bang event as well as for the correct evaluation and selection of optimal substances to be used as a breeder wall in the ITER reactor.

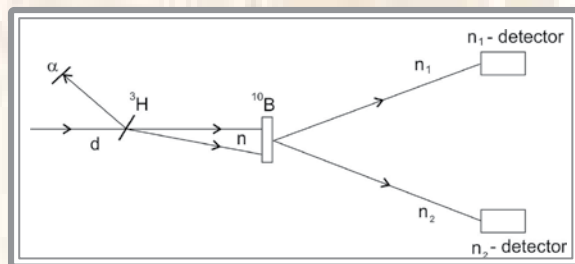


Fig. 6. Investigation of the reaction $^{10}\text{B}(n, 2n)^9\text{B}$.

Studies of sea level change

Sea-level changes over the past 1500 years have been reconstructed based on ^{14}C dating of biological littoral rims from the central Adriatic islands. Distinct phases of relative sea level changes influenced by climate variations were observed.

NEW EQUIPMENT

Detector testing beam line

Facilities for testing detector systems need specially designed vacuum chambers connected to the accelerator beam line for in-beam tests. On the basis of joint efforts by three DEP laboratories and with funding from the FP7 project Particle detectors, one such chamber has been commissioned in 2013. With precise control of detector positioning by xyz translations and rotations in three axes, as well as by using collimated beams of protons and heavier ions over a wide range of energies, it is possible to conduct detector tests in vacuum conditions and in air (using thin membrane exit windows). Installation of this unit at the accelerator facility will greatly increase RBI capabilities for a more active role in international collaborations. This facility will be offered to European scientists for TNA (trans-national access) through future Horizon 2020 projects.



Fig. 7. Detector testing beam line at the RBI accelerator facility.

High resolution PIXE spectrometer

In order to enable studies of chemical effects in x-ray spectra on microscopic sized samples, a new downsized x-ray crystal spectrometer has been constructed. It is based on the excitation of x-rays in tested samples by a proton microbeam, diffraction at the flat crystal and detection of diffraction patterns by a cooled CCD x-ray detector. X-ray spectra are extracted from the CCD images using newly developed routines.

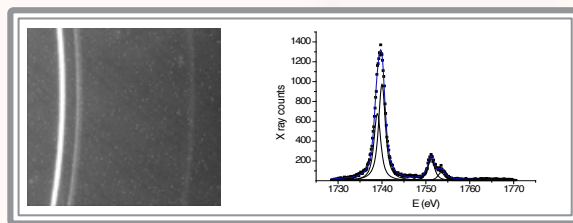


Fig. 8. Diffracted x-rays imaged by CCD of the new high resolution PIXE spectrometer (left) and extracted Si $K\alpha$ x-ray spectrum (right).

EDUCATION

Members of the Division were involved in lecturing at undergraduate and graduate courses at the Faculty of Science at the University of Zagreb, University of Rijeka, and joint studies organized by RBI in cooperation with the Universities of Osijek and Dubrovnik. Four students completed their Ph.D. theses under the leadership of division staff.

PROJECTS

Projects supported by the Ministry of Sciences, Education and Sports

1. Experimental research of the nucleus: nuclear structures and reactions, Suzana Szilner
2. Ion beam interactions and nanostructures, Milko Jakšić
3. Hadronic physics and QCD, Ivan Supek
4. Heavy-ion physics, Zoran Basrak
5. Massive neutrinos and astro-particles: from particle physics to cosmology, Ante Ljubičić

6. Experimental physics at LHC energies, Krešo Kadija
7. Experiments in quantum communication and quantum information, Mario Stipčević
8. Photon-atom interactions and correlations, Tihomir Surić
9. Natural isotopes in investigation of karst environment and dating, Nada Horvatinčić
10. Development and application of nuclear analytical methods, Jasmina Obhodaš
11. Development of the methods for illicit trafficking control, Dario Matika and Davorin Sudac
12. Hadronic physics between the experiments and QCD models, Alfred Švarc
13. Test of special relativity by the Ives-Stilwell type experiment, Saša Blagus
8. Enhancement of Ion Beam Analysis Capabilities Using Novel Detection Systems for PIXE, RBS and STIM, IAEA CRP project No 15988, Stjepko Fazinić
9. Radiation hardness of semiconductors and insulators studied by focused ion beam irradiation and IBIC, IAEA CRP project No. 17051, Milko Jakšić
10. Development of a Reference Database for Particle-Induced Gamma-ray Emission (PIGE) Spectroscopy, IAEA CRP project No. 16688, Iva Bogdanović Radović
11. Search for the new standard model of particle physics at the LHC: from electroweak precision measurements to direct new physics searches, Croatian Science Foundation research grant 09.01/346

Research, developmental and international projects

1. Particle Detectors, Stjepko Fazinić, and Tome Antičić project coordinators, FP7-REGPOT project no. 256783.
2. Support of Public and Industrial Research using Ion beam Technology (SPIRIT), Milko Jakšić, FP7-INFRASTRUCTURES project no. 227012.
3. European Nuclear Science and Applications Research(ENSAR), Milko Jakšić, FP7-INFRASTRUCTURES project no 262010.
4. Hadron Physics 3, Ivan Supek, FP7-INFRASTRUCTURES project no 283286
5. Supporting Postgraduate Research with Internships in industry and Training Excellence (SPRITE), Milko Jakšić, FP7-PEOPLE-2012-ITN project no.317169
6. Studies, training, socio-economical valorization and management of natural, cultural and monumental property for the promotion of the local societies of Latin America (Argentina, Brazil and Mexico) - STRAVAL, FP7- PEOPLE Project, Bogomil Obelić
7. Experimental nuclear physics inputs for thermonuclear runaway, within the collaborative project Physics of compact objects: explosive nucleosynthesis and evolution, Neven Soić, EuroGENESISprogramme of the European Science Foundation
12. Exploiting the LHC Potential to build Collaboration in Science and Technology, Vuko Brigljević, SCOPES Institutional Partnership project (RBI, Paul Scherrer Institute and the University of Sarajevo)
13. ¹⁴C and ¹³⁷Cs in sediments - comparison of methods and application to recent sediments, bilateral project Croatia – Serbia, Ines Krajcar Bronić
14. Synthesis and modification of titanium based nanocomposite materials by ion and laser beam, bilateral project Croatia – Serbia, Iva Bogdanović Radović
15. Enhanced molecular imaging by focused swift heavy ions, bilateral project Croatia-Japan, Tonči Tadić
16. Development of high energy ion microbeam technology for novel applications of diamond, bilateral project Croatia-Japan, Milko Jakšić
17. Studying In-Medium Properties of Strange Particles, Roman Čaplar, RBI and Mile Dželalija, Univ. of Split (Collaboration project Austria-Croatia WIZ 06/2012)
18. Studies of radiation damage in optical fibers and silicon pin diodes, Technical support agreement with KAERI (Korean Atomic Energy Research Institute), Milko Jakšić
19. Influence of climatic and environmental changes on the processes of biologically induced calcite precipitation in Plitvice Lakes, Project with Plitvice National Park, Nada Horvatinčić

20. CERN Axion Solar Telescope (CAST) experiment, Milica Krčmar (International collaboration between RBI and CERN (Switzerland))
21. OPERA collaboration, Mario Stipčević (International collaboration between RBI, CERN (Switzerland) and LNGS (Gran Sasso, Italy))
22. NA61 Collaboration, Krešo Kadija (International Collaboration between RBI and CERN, Switzerland))
23. NA49 Collaboration, Tatjana Šuša (International Collaboration between RBI and CERN, Switzerland)
24. ALICE Collaboration, Tome Antičić (International Collaboration between RBI and CERN, Switzerland)
25. Pierre Auger Observatory (POA), Krešo Kadija (International Collaboration between RBI and POA, Argentina)
26. CMS Collaboration, Krešo Kadija & Vuko Brigljević (International Collaboration between RBI and CERN, Switzerland).
27. MAGIC collaboration, RBI membership through Croatian MAGIC consortium

SELECTED LECTURES

1. Szilner S. Probing nucleon-nucleon correlations via heavy-ion transfer reactions. 25th International Nuclear Physics Conference (INPC 2013), Florence, Italy, June 2-7, 2013.
2. Jakšić M. Radiation tolerance of silicon and diamond detectors exposed to MeV ion beams - characterization using IBIC technique, SPIE Defense, Security, and Sensing 2013, Baltimore, USA, April 29 - May 03, 2013.
3. Jakšić M. Accelerators, ion beams and diamond detectors – between the high energy and materials physics, 8th scientific meeting of Croatian physical society, Primošten, October 6-8, 2013.
4. Horvatinčić N. Carbon isotopes in environmental and palaeoclimate investigation, 23. Hrvatski skup kemičara i kemijskih inženjera. Kutina, Croatia April 21-24, 2013.
5. Đurić S. Diboson studies at CMS. XVII Rencontres de Physique de La Vallée d'Aoste,

La Thuile, Aosta Valley, Italy, February 24 – March 2, 2013.

6. Brigljević V. Measurements of Gauge Boson Self-Interactions at CMS, CERN LHC Seminar, CERN, Geneva, April 30, 2013.
7. Lakić B. Status and perspectives of the CAST experiment. 9th Patras Workshop on Axions, WIMPs and WISPs, Mainz, Germany, June 24-28, 2013
8. Lakić B. IAXO – the future axionhelioscope. 9th Patras Workshop on Axions, WIMPs and WISPs, Mainz, Germany, June 24-28, 2013
9. Fazinić S. Integration of XRF spectrometer for simultaneous and/or complementary use with PIXE at the external ion beam analysis setup. 13th International Conference on PIXE. Gramado, Brasil, March 3-8, 2013
10. Bogdanović Radović I. Formation of semiconductor quantum dots in oxide matrices using MeV ions, 21st International Conference on Ion Beam Analysis, Seattle, USA, June 23-28, 2013.
11. Grilj V. An ultra-thin diamond membrane as a single ion transmission detector at the Zagreb microprobe facility, 21st International Conference on Ion Beam Analysis, Seattle, USA, June 23-28, 2013.

SELECTED ORGANIZED CONFERENCES

1. OPERA Collaboration Meeting, Zagreb, Croatia, September 16-18, 2013 (Jakovčić K, Kliček B and Stipčević M)
2. IAEA Regional Training Course on Dating of Cultural Heritage Artefacts using Nuclear Analytical Techniques, Zagreb, 20 - 24 May 2013, within IAEA Technical Cooperation Project RER/0/034 Enhancing the Characterization, Preservation and Protection of Cultural Heritage Artefacts (Krajcar Bronić I).

SELECTED PUBLICATIONS

1. Chatrchyan S et. al. (CMS Collaboration-RBI: Brigljević V, Đurić S, Kadija K, Luetić J, Morović S, Sudić L) Study of the Mass and

- Spin-Parity of the Higgs Boson Candidate Via Its Decays to Z Boson Pairs. *Phys Rev Lett* **110** (2013a) 081803.
2. Chatrchyan S et. al. (CMS Collaboration-RBI: Brigljević V, Đurić S, Kadija K, Luetić J, Morović S, Sudić L) Measurement of W+W- and ZZ production cross sections in pp collisions at $\sqrt{s} = 8$ TeV. *Phys Lett B* **721** (2013b) 190-211.
 3. Horvat R, Kekez D, Krčmar M, Krečak Z, Ljubičić A. Constraining solar hidden photons using HPGe detector. *Phys Lett B* **721** (2013) 220.
 4. Barth K et al. (CAST Collaboration-RBI: Jakovčić K, Krčmar M, Lakić B, Ljubičić A). CAST constraints on the axion-electron coupling. *JCAP* **1305** (2013) 010.
 5. Agafonova N et al. (OPERA Collaboration-RBI: Jakovčić K, Kliček B, Ljubičić A, Stipčević M). Search for $\nu_\mu \rightarrow \nu_e$ oscillations with the OPERA experiment in the CNGS beam. *J High Energy Phys* **7** (2013) 004.
 6. Adam T et al. (OPERA Collaboration-RBI: Jakovčić K, Kliček B, Ljubičić A, Stipčević M). Measurement of the neutrino velocity with the OPERA detector in the CNGS beam using the 2012 dedicated data. *J High Energy Phys* **1** (2013) 153.
 7. Eudes P, Basrak Z, Sebillé F, de la Mota V, Royer G. Towards a unified description of evaporation-residue fusion cross-sections above the barrier. *Europhys Lett* **104** (2013) 22001.
 8. Ramazani-Moghaddam-Arani A. et al. (BBL Collaboration-RBI: Gasparić I) Spin observables in the three-body break-up process near the quasi-free limit in deuteron-deuteron scattering. *Phys Lett B* **725** (2013) 282.
 9. Szilner S. et al. (Prisma-Clara Collaboration-RBI: Jelavić-Malenica D, Mijatović T, Soić N, Szilner S) The structure of chlorine isotopes populated by heavy ion transfer reactions. *Phys Rev C* **87** (2013) 054322.
 10. Zadro M, Figuera P, Di Pietro A, Fisichella M, Lattuada M, Lönnroth T, Milin M, Ostashko V, Pellegriti M.G, Scuderi V, Stanko D, Strano E, Torresi D. Quasielastic backscattering and barrier distributions for the ${}^6,{}^7\text{Li} + {}^{64}\text{Zn}$ systems. *Phys Rev C* **87** (2013) 054606.
 11. Grilj V, Skukan N, Pomorski M, Kada W, Iwamoto N, Kamiya T, Ohshima T, Jakšić M. An ultra-thin diamond membrane as a transmission particle detector and vacuum window for external microbeams. *Appl Phys Lett* **103** (2013) 243106.
 12. Forneris J, Grilj V, Jakšić M, Olivero P, Picollo F, Skukan N, Verona C, Verona-Rinati G, Vittone E. Measurement and modelling of anomalous polarity pulses in a multi-electrode diamond detector. *Europhys Lett* **104** (2013) 28005.
 13. Šatović D, Desnica V, Fazinić S. Use of portable X-ray fluorescence instrument for bulk alloy analysis on low corroded indoor bronzes, *Spectrochim Acta B* **89** (2013) 7-13.
 14. Fazinić S, Božičević Mihalić I, Mandić L. Influence of chemical environment to the analysis of X-ray spectra of thick pellet samples containing 3d transition metal compounds. *J Anal At Spect* **28** (2013) 1725.
 15. Faivre S, Bakran-Petricioli T, Horvatinčić N, Sironić A. Distinct phases of relative sea level changes in the central Adriatic during the last 1500 years – influence of climatic variations? *Palaeogeography, palaeoclimatology, palaeoecology*. **369** (2013), 163.
 16. Valković V, Sudac D, Obhodas J, Eleon C, Perot B, Carasco C, Sannić G, Boudergui K, Kondrasovs V, Corre G, Normand S, Woo R, Bourbotte J.M. The use of alpha particle tagged neutrons for the inspection of objects on the sea floor for the presence of explosives. *Nucl Instr Meth A* **703** (2013) 133.

Book chapter

1. Barešić J: Recent lake sediments, STRAVAL case study: Croatia - selected site: Plitvice Lakes National Park; Obelić B, Krajcar Bronić I (eds), Barcelona. Marie Curie Actions - IRSES Project STRAVAL, 2013. pp 48-55.
2. Horvatinčić N: Tufa and lake sediment formation, STRAVAL case study: Croatia - selected site: Plitvice Lakes National Park / Obelić B, Krajcar Bronić I (eds). Barcelona. Marie Curie Actions - IRSES Project STRAVAL, 2013. pp 34-41.

3. Obelić B: Introduction to Plitvice Lakes National Park, STRAVAL CASE STUDY: CROATIA - Selected site: PLITVICE LAKES NATIONAL PARK / Obelić B, KrajcarBronić I (eds). Barcelona. Marie Curie Actions - IRSES Project STRAVAL, 2013. pp 7-24.
4. Obelić B, Horvatinčić N: Geochronology, STRAVAL case study: Croatia - selected site: Plitvice Lakes National Park, Obelić B, KrajcarBronić I (eds). Barcelona. Marie Curie Actions - IRSES Project STRAVAL, 2013. pp 42-47.



DIVISIONAL ORGANIZATION

Head: Branko Šantić

The Division of Materials Physics (ZFM) consists of the following laboratories:

- ⇒ Laboratory for Semiconductors, Branko Pivac
- ⇒ Laboratory for Thin Films, Nikola Radić
- ⇒ Laboratory for Molecular Physics, Mile Ivanda



TOP ACHIEVEMENTS

A new mechanism for tuning the growth properties of Ge quantum dot lattices is found

Self-assembled growth of Ge quantum dot lattices in oxide matrices prepared by the quite simple magnetron sputtering deposition method allows the preparation of a variety of structures tunable by their shape, size and arrangement. The driving mechanism for the self-assembly was attributed to the surface morphology features originating from the quantum dots' growth. It has been shown that the matrix type is another critical factor

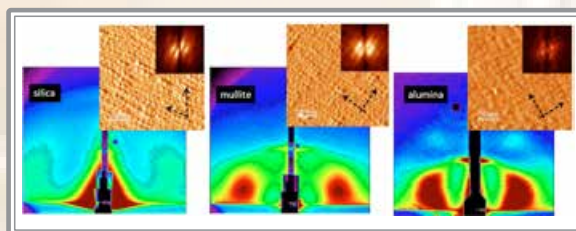


Fig. 1. Tuning the type of Ge quantum dot ordering by matrix composition.

OVERVIEW OF THE DIVISION

The main topics of the research are in the field of basic science of materials, particularly semiconductors, thin films and molecular physics. Besides, various applied oriented investigations and activities are also present. Several advanced experimental setups for the growth of samples and complex structures exist in the department. Various experimental techniques are used for the characterization of samples and for the explanations of their properties on molecular and atomistic scale. Some scientists are involved in theoretical modeling and numerical simulations, either in order to explain experimental results, or to suggest new directions of research and/or applications. Department members are active in numerous joint research projects, both on national and international level.

that enables the control of the self-assembly process and the tuning of the ordering type and degree of regularity of quantum dot systems. The obtained results are relevant for understanding and tailoring of the self-assembled growth of quantum dot lattices in amorphous systems (Buljan et al., 2013).

Tuning the Microstructure of γ -Ba₄Nb₂O₉ Polymorph Prepared from Single-Molecular Precursor

New procedure for preparation of γ -Ba₄Nb₂O₉ from a single-molecular metal-organic precursor was developed. The method involves a high temperature treatment of the precursor and a controlled cooling of the product. Phase composition and morphology were controlled by (i) holding time at the given temperature and (ii) the cooling rate. The HT polymorph has been successfully retained at RT. The desired crystallite size in the nanoscale regime (~5 to 20 nm) can easily be tuned (Popović et al., 2013).

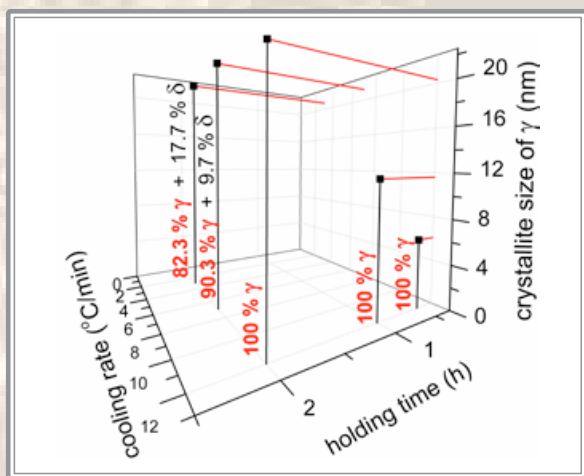


Fig. 2. Correlation of the cooling rate and the holding time to the crystallite size of γ -Ba₄Nb₂O₉.

Phase matching between coated microsphere and tapered fiber

Using a sol-gel deposition process, we managed to gradually change the effective refractive index of silica microspheres by coating them with a material with a refractive

index higher than the refractive index of silica. The film used for coating was 70 SiO₂ - 30 HfO₂ doped with Er³⁺ ions. We have studied the coating dependence of the intensity of luminescence of the whispering gallery modes inside the micro-resonators, and have found that the luminescence intensity increases linearly with the thickness of the coating. From measurements of the free spectral range, we concluded that the observed modes correspond to the fundamental ($n = 0$) modes. We have considered the role of phase matching in the coupling between whispering gallery modes in the microresonator and the propagation mode in the tapered fiber used for excitation, and have concluded that the observed modes correspond to strongly delocalized azimuthally ($m < l$) modes, out of which at least one is always quasi-phase matched with the propagating mode in the tapered fiber. This means that, no matter how high the refractive index of the coating layer is, it is always possible to excite the microresonator using a fiber taper with very high efficiency (Ristić et al., 2013).

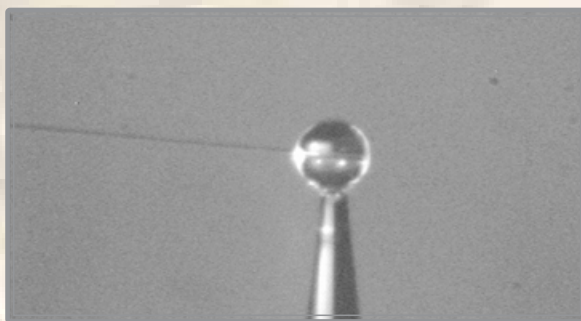


Fig. 4 Optical microscopy image of the microsphere and tapered fiber.

In situ Raman spectra recorded at phase transition temperatures

The aim of the work is the study of the phase transition from the tetragonal ferroelectric to the cubic paraelectric phase in polycrystalline BaTiO₃ nanorods that is crucial for possible application. Nanorods consist of tetragonal nanocrystals with inter-grown nanolamellas of the hexagonal phase. Ra-

man spectroscopy showed that nanorods underwent a diffuse phase transition from tetragonal to cubic phase with respect to the temperature, whereas the final phase-transition temperature was shifted to higher values compared to that typically expected for BTO (Gajović et al., 2013)

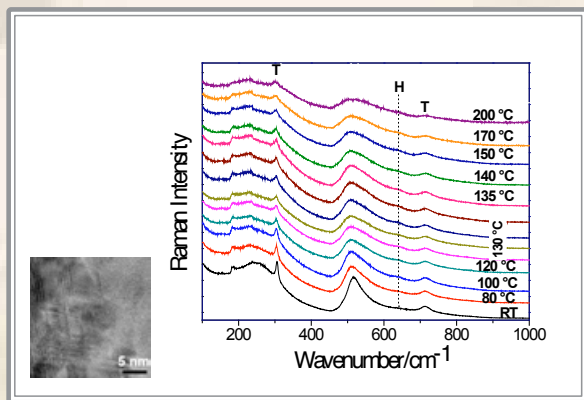


Fig. 3. HRTEM of hexagonal phase responsible for stabilization of tetragonal phase at temperatures higher than expected phase transition

Disorder in the Ta_xN thin films and Raman spectroscopy

Ta_xN alloy systems are used in a variety of applications and some of them are as compact thin-film resistors or diffusion barriers in copper interconnects on Si chips. Analyses of the properties of these layers are usually performed on crystalline sapphire substrates, which are, when compared to the standard silicon wafers, expensive and have more structural and surface defects. First order Raman absorption in materials with the rock salt crystal structure is forbidden. Its appearance in real crystals results from the presence of vacancies and other defects. For Ta_xN polycrystalline thin films, we found that imperfections that reduce the coherence length contribute to the appearance of the first order Raman spectrum. This investigation enables us to better understand the anomalous concentration dependence of the resistivity of Ta_xN polycrystalline thin films fabricated using reactive sputtering (Očko et al., 2013).

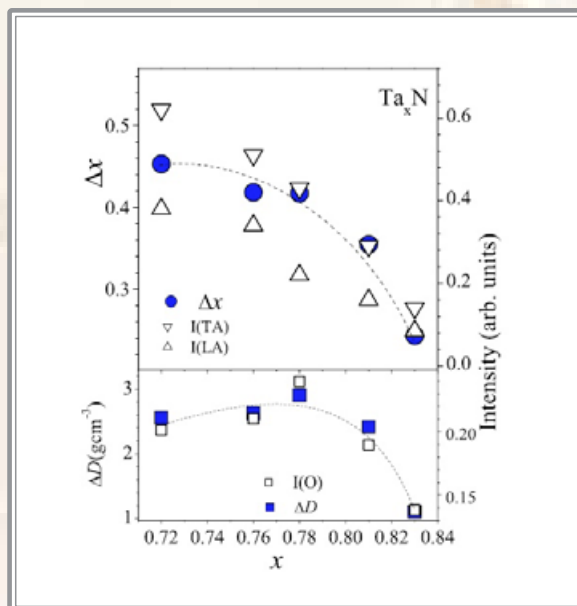


Fig. 4. Comparison of x-ray and Raman spectroscopy data of Ta_xN polycrystalline thin films in dependence on Ta content.

Vibrational studies of cobalt(II) complexes with 3- hydroxypicolinic acid

The Raman, infrared and theoretical analysis is given for complex $cis-[Co(3-OHpic)_2(4-pic)_2]$ (3) (py = pyridine ; 4-pic = 4-picoline or 4-methylpyridine). The calculated spectra agree very well with the presented experimental findings. The same vibrational calculations also reveal insignificant influence of $H \rightarrow CH_3$ substitution for the spectroscopic characterization of the complex (Furić et al., 2013).

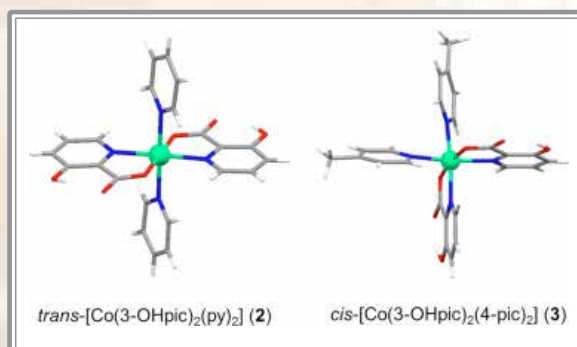


Fig. 5. Trans and cis conformation of the complex

Vibrational dynamics of gases aminopropylsilanetriol

Raman spectrum of aminopropylsilanetriol (APST) in gas phase has been recorded at room temperature in macro chamber utilizing two-mirror technique over the sample tube. Unlike predominantly trans molecular conformation in condensed phase, the spectra of vapor show that the molecules are solely in gauche conformation with intramolecular hydrogen bond $N \cdots H-O$ which reduces the molecular energy in respect to trans conformation by 0.152 eV. The assignment of the molecular spectra based on the DFT calculation is presented. The strong vibrational bands at 354 cm^{-1} , 588 cm^{-1} and 3022 cm^{-1} are proposed for verifying the existence of the ring like, hydrogen bonded structure. Special attention was devoted to the high frequency region, where hydrogen bond vibrations are coupled to stretchings of amino and silanol groups (Volovšek et al., 2013).

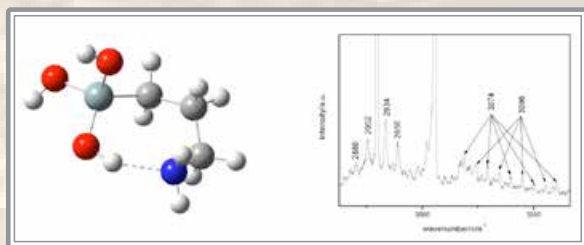


Fig. 6. Aminopropylsilanetriol with its Raman spectrum

New routes in preparation of porous silicon

Porous silicon (PSi) samples were prepared by galvanostatic electrochemical anodization of epitaxial silicon, polycrystalline silicon and silicon on insulator layers. Epitaxial silicon layers of n-type and $\langle 111 \rangle$ orientation grown on n-type $\langle 111 \rangle$ oriented silicon substrates were anodized as a function of concentration of 48 % HF in ethanol solution and anodization time. Electrical resistivities of the epitaxial layers and of the silicon substrate were 2 and $0.015\text{ }\Omega\text{cm}$, successively. Within the obtained porous silicon layers the

micro- and nano-pores of different sizes in dependence on HF concentration and anodization time were obtained (Ivanda et al., 2013).

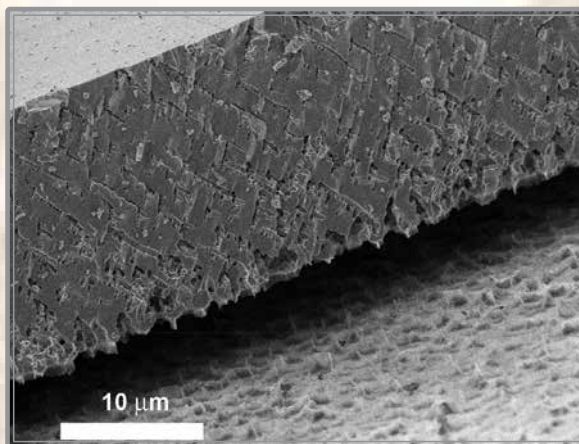


Fig. 7. Thin layer of porous silicon obtained by galvanostatic electrochemical anodization of epitaxial silicon.

EDUCATION

Members of the Division of Materials Physics were involved in teaching of 10 undergraduate and 4 postgraduate courses of physics and related topics at the Faculty of Sciences, Faculty of Electrical Engineering and Computing, Faculty of Chemical Engineering and Technology in Zagreb and elsewhere.

AWARDS

Maja Buljan, Donation of *Adris group* for the project “*Solar cells based on self-assembled quantum dots in glasses*”, 2013-2015.

Vedran Đerek, Ernst Mach Research Award for the project “Photovoltaic effects in hybrid silicon nanodevices” (6 month doctoral research at Linz Institute of Organic Solar Cells, Linz, Austria).

PROJECTS

Research program supported by the Ministry of Science, Education and Sports

1. Advanced materials and applications for energy conversion and storage, Branko Pivac

Research projects supported by the Ministry of Science, Education and Sports

1. Synergy of nanophases and nanocomposites, Maja Buljan
2. Basic properties of nanostructures and defects in semiconductors and dielectrics, Branko Pivac
3. Doped optoelectronic and ceramic nanomaterials, Biserka Gržeta
4. The thin film silicon alloys on the amorphous to crystalline transition, Davor Gracin
5. Thin Films of Novel Amorphous or Nanostructured Materials, Nikola Radić
6. Semiconductor materials for optoelectronics and nanotechnology, Branko Šantić
7. Physics and application of nanostructures and bulk matter, Mile Ivanda
8. Organizational processes and optical interactions in condensed molecular systems, Dubravko Risović

Research, developmental and international projects

1. FP-7 NanoPV—Nanomaterials and nanotechnology for advanced photovoltaics, B. Pivac
2. Multifunctional complex metal tellurates: Structure-property relationship study (UKF project 1.370.000,00 kn), I. Đerđ
3. *Solar cells based on self-assembled quantum dots in glasses* (PI M. Buljan, PI), Donation of *Adris group*, 2013-2015.
4. Nanoporous multifunctional materials - Toward novel multiferroic (J. Popović, PI) (Croatian-German bilateral project 2013-2014)
5. XBroad-program for microstructural determination from powder diffraction data (J.

- Popović, PI) (Croatian Academy for Sciences and Arts project 2013)
6. Doping semiconductor nanocrystals by neutron transmutation method, I. Capan (Bilateral, Croatia-Slovenia)
7. Comparison between electrical and structural properties of doped germanium nanocrystals, I. Capan (Bilateral, Croatia-Germany)
8. New Nanostructural Materials for Thermoelectrics, M. Ivanda (Bilateral, Croatia-Slovenia)
9. COST Action MP 0901: Designing Materials for Nanodevices – from Theory to Practice, I. Capan
10. COST Action MP0904, Single- and multiphase ferroics and multiferroics with restricted geometries (SIMUFER), A. Gajović
11. COST Action MP 1302, NanoSpectroscopy, M. Ivanda
12. New inorganic-organic hybrid materials: elucidation of structure by combining powder diffractometry and optimization of geometry applying DFT calculation (Bilateral, Croatia-France), I. Đerđ
13. Sol-gel synthesis and characterization of TiO₂ nanostructures with improved electrical conductivity (Bilateral, Croatia-Germany), I. Đerđ

SELECTED INVITED LECTURES

1. Pivac B (2013) Challenges in designing/building advanced photovoltaics. Advanced workshop: New trends in nanophysics and solar energy conversion, Bucharest, Romania, September 23-25, 2013.
2. Buljan M (2013) Self-assembly of semiconductor quantum dots in amorphous dielectric matrices. 19th International Vacuum Congress (IVC-19) & International Conference on Nanoscience and Technology (ICN+T 2013) & 15th International Conference on Solid Surfaces (ICSS-15), Paris, France, September 09-13, 2013.
3. Popović J (2013). Nanocrystalline metal oxides: synthesis, characterization and application. The twenty-second Croatian-Slovenian crystallographic meeting - CSCM22, Biograd, Hrvatska, June 12-16, 2013.

SELECTED ORGANIZED CONFERENCES

1. 19th International Vacuum Congress (IVC-19) & International Conference on Nanoscience and Technology (ICN+T 2013) & 15th International Conference on Solid Surfaces (ICSS-15), Paris, France, September 09-13, 2013. (Radić N Organizing Committee Vice-chair)

SELECTED PUBLICATIONS

1. Buljan M, Jerčinović M, Siketić Z, et al. Tuning the growth properties of Ge quantum dot lattices in amorphous oxides by matrix type. *J Appl Crystallogr* 46 (2013) 1490.
2. Popović J, Vrankić M, Jurić M. Tuning the Microstructure of gamma-Ba₄Nb₂O₉ Polymorph Prepared from Single-Molecular Precursor. *Cryst Growth Des* 13 (2013) 2161.
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13. Buljan M, Radić N, Ivanda M, et al. Ge quantum dot lattices in Al₂O₃ multilayers. *J Nanopart Res* 15 (2013) 1485.

BOOK CHAPTERS

1. Ivanda M, Balarin M, Gamulin O, Đerek V, Ristić D, Musić S, Ristić M, Kosović M. Porous Silicon by Galvanostatic Electrochemical Anodisation of Epitaxial Silicon, Polycrystalline Silicon and Silicon on Insulator Layers; Advanced sensors for safety and security, Vaseashta, Ashok; Khudaverdyan S (ed.), London: Springer, 2013. p. 303-320.
2. VACUUM 98 (2013) Elsevier / Special Issue JVC14/EVC12/AMDVG11/CroSloVM19, June 4-8, 2012, Dubrovnik, Croatia, Proceedings, Guest Editors: Radić N, Milošević S, Pivac B

DIVISIONAL ORGANIZATION

Head: Hrvoje Zorc

The Division of Laser and Atomic R&D (Zavod za laserska i atomska istraživanja i razvoj) consists of the following laboratories:

- ⇒ Laboratory of Thin Films and Optics, Vesna Janicki
- ⇒ Multipurpose workshops, Marijan Horvatiček



OVERVIEW OF THE DIVISION

The mission of the Division is to expand and strengthen our knowledge in the field of imaging and non-imaging optics, photonics and the fundamentals of optical thin films. In addition, activities are directed to the application of basic disciplines in the field of national security.

The Division is currently developing several strategic projects. These include modelling of thin films mixtures using effective medium theories, research on the plasmonic properties of metallic nanoclusters, the use of plasmonic materials in optical multilayer design, characterization and modelling of very thin metallic layers, sparse component analysis and tensor factorization approaches to feature extraction from multispectral images and protein and/or gene expression levels with applications in disease (cancer) diagnosis

and biomarker identification, nonlinear decomposition of multichannel medical images with application in contrast enhancement of multi-phase CT image and multispectral images in pathology, an independent component analysis based approach to dictionary learning for efficient representations of the images of natural scenes with applications in filling-in missing values as well as denoising of images corrupted by salt and pepper noise and consensus-based regression with applications in prediction of anti-tumor activity of virtual chemical compounds.

The Division participated in one strategic project in the field of national security, together with an industry partner and in cooperation with the Croatian Ministry of Defence.

TOP ACHIEVEMENTS

Ellipsometric characterization of plasmonic nanocomposites

Research on the optical characterization of metal-dielectric composites with plasmonic properties continued in 2013. Our know-how in modeling the dielectric function

wavelength dependence extracted from ellipsometric measurements has been used to investigate novel composites. In particular, we investigated the application of such composites to increase the anti-reflective properties of solar cells. The proposed application structure consists of a film made of a porous TiO₂ matrix containing Au nanoparticles. It has been shown that by controlling the porosity and particle size and concentration, the reflectance of a silicon substrate coated by such a plasmonic layer decreases to practically zero over a broad range of wavelengths around the localized surface plasmon resonance. Ellipsometric analysis of these structures allowed for an understanding of the contribution of gold nanoparticles and pores to the anti-reflective behaviour (Sancho-Parra et al., 2013).

Optical forces in nanoparticle systems

Algorithms previously developed for calculating multiple scattering in systems of nanoparticles have been extended to calculate optical forces acting on particles. Optical forces result from the transfer of light momentum to particles and are the key element of optical tweezers. Our first results have been applied to the in-vivo study of molecular motors. In particular, we simulated the influence of lipids located in the vicinity of a vesicle trapped by optical tweezers. In addition, we theoretically studied the possibility of trapping small dielectric objects by using strongly localized evanescent fields that can be generated in plasmonic clusters.

Design of optical metasurfaces

Artificial electromagnetic materials or metamaterials have received a lot of attention due to the possibility to almost arbitrarily mold the flow of light, thus opening the path to unique applications such as super-resolution or cloaking. However, bulk

metamaterials have intrinsic losses that drastically limit their performance. Recently, the concept of a metasurface, as 2D metamaterial, has been proposed as a promising alternative where the impact of losses is minimized. We have initiated research in this area, proposing a new concept for an optical metasurface that could act as a double-boundary condition, i.e., with vanishing normal components of the displacement and magnetic fields. Such a metasurface could in principle be obtained by properly structuring a plasmonic thin film (Figure 1).

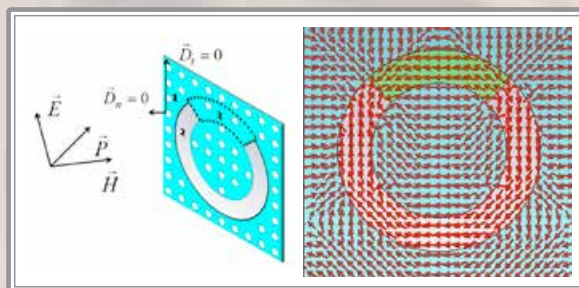


Fig. 1. Scheme of the proposed optical double-boundary metasurface unit cell (left) and electric field distribution at resonance (right)

Blind data analysis

Research efforts were focused on methods for unsupervised (a.k.a. blind) data analysis with emphasize on methods for sparseness constrained factorization of (multi-) linear and nonlinear mixture models in reproducible kernel Hilbert spaces (RKHS). Novel algorithms were derived and applied to the following problems: (i) extraction of pure components from a small number of mixtures of mass spectra; (ii) variable (feature) selection for non-invasive diagnosis of melanoma and disease diagnosis from genomic and/or proteomics expression profiles (Kopriva et al., 2013).

EDUCATION

Members of the LAIR lead BSc, MSc and PhD theses at the University of Applied Sciences Velika Gorica, Karlovac University of

PROJECTS

Projects supported by the Ministry of Science, Education and Sports

1. Analysis of multispectral data, Ivica Kopriva
2. Optical properties of nanostructured films, Hrvoje Zorc

Projects supported by the Croatian Science Foundation

1. Analysis of nonlinear components with applications in chemometry and pathology, Ivica Kopriva

SELECTED INVITED LECTURES

1. Janicki V (2013): Optical coatings with metal island films. COST Workshop on characterization of semiconductor nanostructures; the role of defects, Zagreb, Croatia, December 2-4, 2013.
2. Sancho-Parramon J (2013): Ellipsometric characterization of thin films containing metal nanoparticles. COST Workshop on characterization of semiconductor nanostructures;

the role of defects, Zagreb, Croatia, December 2-4, 2013.

3. Lončarić M (2013): Plasmonics of noble metal nanoparticles, 20th International Scientific Meeting on Vacuum Science and Techniques, Jeruzalem, Slovenia, May 9-10, 2013.
4. Kopriva I (2013): Sparse component analysis - applications in multichannel medical imaging and bioinformatics, 2013 IEEE Signal Processing Society Summer School on Biomedical Image Processing and Analysis, Dubrovnik, Croatia, June 9, 2013.
5. Kopriva I (2013): Tensor factorizations-applications in multichannel medical imaging and bioinformatics, 2013 IEEE Signal Processing Society Summer School on Biomedical Image Processing and Analysis, Dubrovnik, Croatia, June 10, 2013.

SELECTED PUBLICATIONS

1. Kopriva I, Jerić I, Brkljačić L. Nonlinear Mixture-wise Expansion Approach to Underdetermined Blind Separation of Nonnegative Dependent Sources. *J Chemom* **27** (2013) 189.
1. Pedrueza E, Sancho-Parramon J, Bosch S, Valdes J L, Martinez-Pastor J P. Plasmonic layers based on Au-nanoparticle-doped TiO₂ for optoelectronics: structural and optical properties. *Nanotechnology* **24** (2013) 065202.



DIVISIONAL ORGANIZATION

Head: Tomislav Šmuc

The Division of electronics consists of two laboratories and one research group:

- ⇒ Laboratory for information systems, Dragan Gamberger
- ⇒ Laboratory for stochastic signals and processes research, Branka Medved Rogina
- ⇒ Computational biology and bioinformatics group, Tomislav Šmuc



neering and Computing, the Faculty of Sciences and School of Medicine of the University of Zagreb.

TOP ACHIEVEMENTS

Knowledge technologies and computer science applications

Participation in a study on large scale protein-function prediction

To understand the current deluge of genomic data, computational approaches for gene functional annotation are invaluable. We have participated in a world-wide large scale protein-prediction study whose results have been published recently (Radivojac et al., 2013). Our specific role in this collaboration used a novel computational pipeline for protein function annotation based on phyletic profiles of nearly a thousand prokaryotic genomes and state-of-the-art multi-label classification algorithm.

Machine learning in complex systems/networks

Research in the field of complex systems/networks represents a new application area

OVERVIEW OF THE DIVISION

The mission of the Division of Electronics is the development of techniques and approaches capable of tackling data and information overload, a common problem for most scientific disciplines and contemporary technology environments. We develop techniques and approaches that blend signal processing, data handling, machine learning and data mining, with modern programming paradigms and knowledge technologies. Novel topics include machine learning and data mining in a complex networks setting and implementation of machine learning algorithms on programmable hardware. Our main application disciplines include biomedical engineering, biology (genomics/proteomics), economics and social sciences. The Division has 15 staff members of which six are PhD students.

The members of the Division are involved in lecturing at the Faculty of Electrical Engi-

for the Division. We participate in two high profile FET projects related to development of new mathematical and computational frameworks for studying complex systems via networks formalism: FOC (Forecasting Financial Crisis) and MultiPlex (Foundational Research on Multilevel Complex Networks and Systems). Within the FOC project, we have developed a novel index reflecting cohesiveness of a typically large corpus of texts. We have shown that for financially related news our index (NCI-news cohesiveness index) is related to global financial market volatility. NCI is a big-data index suitable for comprehensive text processing pipelines such as NewStream developed by the Jozef Stefan Institute as part of the same project. Another topic of interest is related to studying contagion or epidemic processes on networks, more specifically determination of the source of epidemics from partially observed realization of epidemics. We have extended our recently developed statistical framework for the estimation of epidemic sources in arbitrary networks with new algorithms, and studied the limits of source detectability in different contagion process regimes.

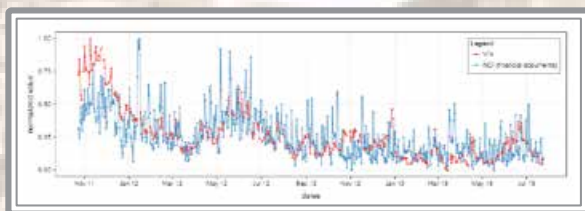


Fig.1. News Cohesiveness Index and VIX (Implied volatility index of S&P500 index) showing highly correlated behavior.

Key phrase extraction and opinion mining

Work on key-phrase extraction algorithms based on semantic technologies was started in collaboration with Jan Šnajder (Faculty of Electrical Engineering and Computing, University of Zagreb). A method for extraction of aspect-oriented opinion data from product reviews was developed in collaboration with Goran Glavaš and Jan Šnajder (Faculty of

Electrical Engineering and Computing, University of Zagreb). The associated dataset, annotated with linguistic data, is available at: <http://takelab.fer.hr/data/cropinion/>

Using FPGAs to accelerate data mining tasks

FPGAs have proven to be an effective platform for accelerating a wide range of machine learning algorithms, most notably those whose core can be easily expressed as a dataflow graph (e.g. SVM, k-means clustering). The dataflow model of computing represents a compute task as a series of transformations on a stream of data elements (e.g. individual elements of matrices or vectors). We explore use of the dataflow computational model on one of the most commonly used class of data mining algorithms – decision tree learning. A widely popular decision tree learning algorithm, C4.5, using the commercial FPGA acceleration system Maxeler Vectis was implemented. The implementation is a careful partition of compute tasks into software and hardware parts which are finely coordinated to provide maximum performance.

Platform for embedded systems learning



The first year of the three-year E2LP project (<http://www.e2lp.org/>) ended in August 2013, with successful comple-

tion of the E2LP Startup-kit. The main idea behind the project is to provide a unified platform which will cover a complete process for embedded systems learning. A modular approach is considered for skills practice through supporting individualization in learning. The E2LP startup-kit is a compilation of laboratory exercises intended to be run on an E2LP board. In this part of the project we had the role of work package leader in charge of de-

fining/implementing the library of laboratory exercises as well as being producers of a set of exercises. We have provided exercises in the field of FPGA based computing and signal processing.

EDUCATION

Educational activities in 2013 encompassed providing course lectures at the undergraduate and post-graduate level at the Faculty of Electrical Engineering and Computing („Algorithms and Data Structures“, S. Ristov; „Optical Networks“, B. Medved Rogina), the Faculty of Sciences („Machine Learning“, T. Šmuc) and School of Medicine of the University of Zagreb („Knowledge Discovery“, D. Gamberger).

PROJECTS

Projects supported by the Ministry of Science, Education and Sport

1. Machine Learning Algorithms and their Application, Dragan Gamberger
2. Computational Intelligence Methods in Measurement Systems, Ivan Marić
3. Real Life Data Measurement and Characterization, Branka Medved Rogina
4. Machine Learning of Predictive Models in Computational Biology, Tomislav Šmuc

Research, developmental and international projects

1. FOC - Forecasting Financial Crises (EU-FP7 FET Project) Tomislav Šmuc, Dragan Gamberger.

2. Multiplex – Foundational Research on Multi-level Complex Networks and Systems (EU-FP7 FET Project), Tomislav Šmuc, Dragan Gamberger.
3. Embedded computer engineering learning platform – E2LP, EU FP7 STREP, Branka Medved Rogina, WP leader.

SELECTED INVITED LECTURES

1. Gamberger D (2013) Descriptive modeling in social sciences, Knowledge Technologies Symposium on Machine Learning and Computational Creativity, Institute Jozef Stefan, Ljubljana, Slovenia, July 4, 2013.

SELECTED ORGANIZED CONFERENCES

1. International Workshop: Rule learning algorithms and their applications, Zagreb, Croatia, February 15, 2013.

SELECTED PUBLICATIONS

1. Radivojac P et al. A large-scale evaluation of computational protein function prediction. *Nat Methods* **10** (2013) 221.
2. Levatić J, Ćurak J, Kralj M, Šmuc T, Osmak M, Supek F. . Accurate Models for P-gp Drug Recognition Induced from a Cancer Cell Line Cytotoxicity Screen. *J Med Chem* **56** (2013) 5691.
3. Marić I. Optimization of self-organizing polynomial neural networks, *Exp Syst Appl* **40** (2013) 11.



DIVISIONAL ORGANIZATION

Head: Aleksandar Sablić

The Division of Physical Chemistry (ZFK) consists of the following laboratories:

- ⇒ Laboratory for Chemical Kinetics and Atmospheric Chemistry, Branka Kovač
- ⇒ Theoretical Chemistry Group, Nađa Došlić
- ⇒ Laboratory of Chemical and Biological Crystallography, Marija Luić
- ⇒ Laboratory for Magnetic Resonances, Boris Rakvin
- ⇒ Laboratory for Synthesis and Processes of Selfassembling of Organic Molecules, Ivan Habuš



chemistry, modelling of physical and chemical processes as well as in peptide and protein research. A significant number of articles were published in high ranking journals such as: *Angewandte Chemie International Edition*, *Journal of Physical Chemistry Letters*, *Inorganic Chemistry*, *Journal of Organic Chemistry*, *Nucleic Acids Research*, *Journal of Computational Chemistry*, *Physical Chemistry Chemical Physics*, *Dalton Transaction*, *Structure*, and *CrystEngComm*. About half of the published works were the result of domestic and international collaborations. A number of fruitful international collaborations demonstrate a strong presence of the Division in the European Research Area. Furthermore, division members were successful in securing new competitive grants through the ERC program (Biological membranes in action: A unified approach to complexation, scaffolding and active transport, Ana-Sunčana Smith) and the UKF program (Time resolved photoelectron spectroscopy as a probe for ultrafast excited state dynamics, Nađa Došlić). Division members also contributed extensively (about 30 courses) to undergraduate and graduate education in Croatia.

OVERVIEW OF THE DIVISION

The mission of the Division of Physical Chemistry is to discover, exploit, and disseminate fundamental knowledge in the fields of protein science, coordination chemistry, spectroscopy, and computational and theoretical chemistry, in order to emerge as an internationally recognized Centre of Excellence in selected areas of molecular research.

In 2013 members of the Division published nearly 50 research articles in atmospheric chemistry, chemical kinetics, structural chemistry, theoretical and computational

TOP ACHIEVEMENTS

Separation of solid dicarboxylic acid isomers by molecular recognition and mechanochemistry

A new method, based on the principles of supramolecular chemistry is presented here, where a flexible receptor is used for supramolecular recognition and selective binding of solid maleic acid from a vast excess of fumaric acid and/or different isomers of benzenedicarboxylic acids (Užarević et al., 2013). The receptor adapted its geometry in order to create a specific binding site for each tested isomer (Figure 1), but in the presence of maleic acid, the receptor:hydrogenmaleate complex is formed exclusively. Most importantly, the recognition and selective binding of isomers was conducted in the solventless environment of the grinding jar during the milling process. This type of recognition is a largely unexplored area of research and it highlights the potential of this methodology for green and waste-reducing separation technologies.

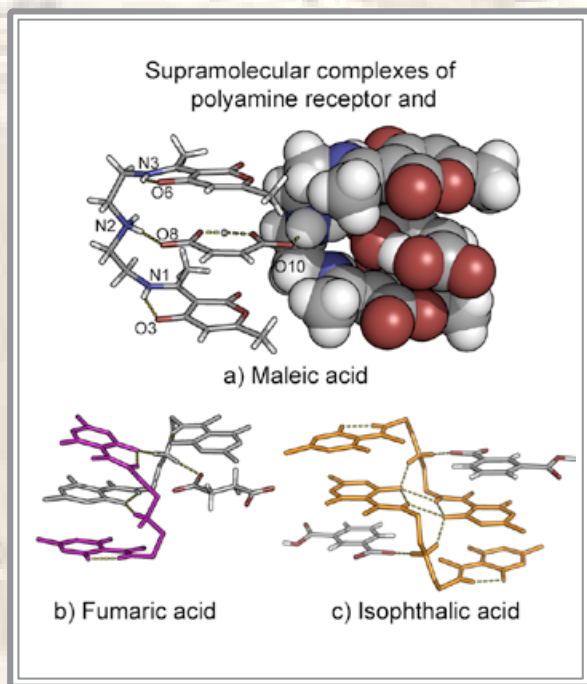


Fig. 1. Supramolecular complexes of polyamine receptor and (a) maleic acid, (b) fumaric acid and (c) isophthalic acid.

Cyclopalladation of azobenzenes: kinetics and mechanisms

The well known ability of azobenzene ligands to undergo cyclopalladation has been exploited to produce dicyclopalladated complexes. Special attention was paid to the 4,4'-substituents on the azobenzene ligand which play an important role in the structural and photophysical properties of dipalladated azobenzenes as well as in the kinetics of their cyclopalladation, Figure 2. The effect of different 4,4'-substituents on the formation rate of mono- and dicyclopalladated azobenzenes was studied by UV-vis spectroscopy. The kinetic results supported by the Hammett correlations demonstrated a strong effect of different 4,4'-substituents on the formation rate of mono- and dicyclopalladated azobenzenes. Experimental findings rationalized by quantum-chemical calculations strongly suggest that both cyclopalladations of azobenzenes proceed via two successive steps: the first is related to the formation of adducts, which is followed by the formation of the final (mono- or di-) cyclopalladated product (Juribašić et al., 2013).

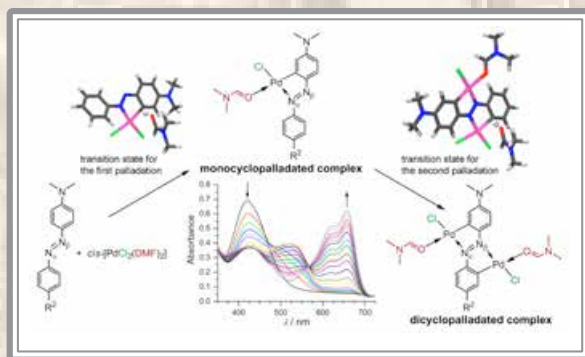


Fig. 2. Cyclopalladation of azobenzenes.

Efficient buffer-mediated control between free radical substitution and proton-coupled electron transfer

A remarkable buffer-mediated control between free-radical substitution (FRS) and

proton-coupled electron transfer (PCET) is demonstrated for the reaction between iodoethane and the α -hydroxyethyl radical in neutral aqueous solution in the presence of bicarbonate or phosphate buffer. Addition of a basic buffer anion is indispensable for the reaction to occur and the competition between the two channels depends subtly on its proton accepting affinity, with FRS being the dominant channel in phosphate containing solutions and PCET in bicarbonate containing solutions. Unlike the former, the latter channel sustains a chain-like process which significantly enhances dehalogenation. The present systems furnish an example of the novel PCET/FRS dichotomy, as well as insights into possibilities of its efficient control (Ljubić et al., 2013).

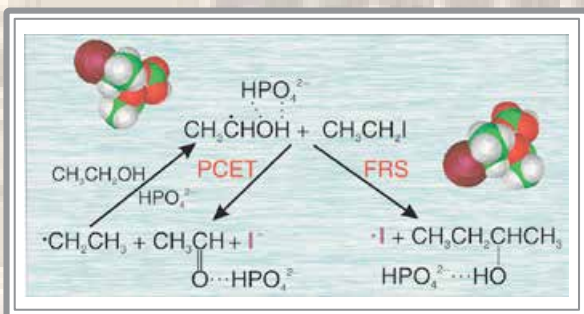


Fig 3. Competition between free radical substitution and proton-coupled electron transfer in the reaction of the α -hydroxyethyl radical with iodoethane in buffered aqueous medium.

Structural investigation of protein-protein complexes

Recently a new family of enzymes, the amino acid:[carrier protein] ligase (aa:CP ligases) were discovered. These enzymes are highly similar to class II aminoacyl-tRNA synthetases (aaRSs), but aminoacylate different substrates. aaRSs aminoacylate tRNA supply the building blocks for ribosomal translation, while aa:CP ligases transfer activated amino acids to the phosphopantetheine group of small carrier proteins. Comprehensive crystallographic studies of the aa:CP ligases complexed with carrier proteins revealed how the conserved class II aaRS catalytic core

can adapt to a novel function through minor structural alterations. A new and unforeseen mode of macromolecular interactions was described and a mechanism of catalytic reaction proposed (Močibob et al., 2013).

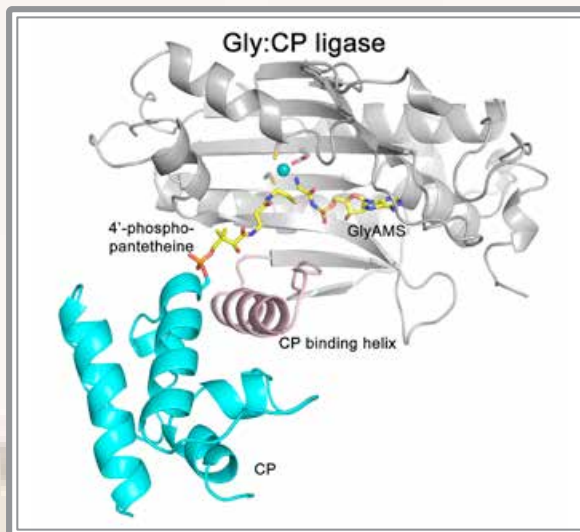


Fig 4. Protein-protein interaction between glycyl-CP ligase 1 from *Bradyrhizobium japonicum* and its cognate carrier protein.

Lamellar to hexagonal columnar liquid crystalline phase transition in a catanionic surfactant mixture

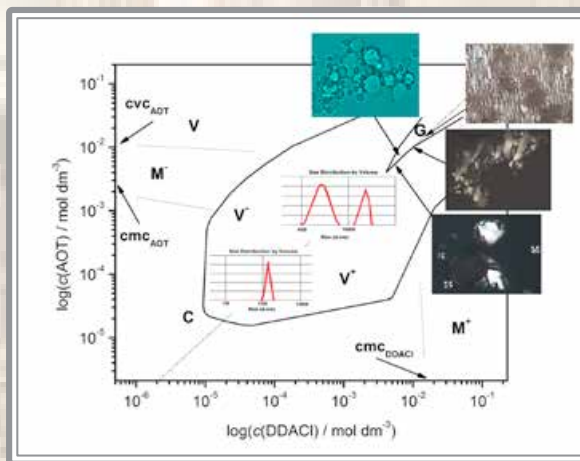


Fig 5. Phase behavior of the DDACl/AOT/H₂O system at high water content obtained after 24 hours at 298 K.

Phase transitions from a dispersed lamellar to hexagonal liquid crystalline phase have been investigated in a catanionic surfactant mixture formed by mixing a single tailed cati-

onic surfactant, dodecylammonium chloride, with a double tailed anionic surfactant, sodium bis(2-ethylhexyl) sulfosuccinate. The transition proceeds through the processes of vesicle aggregation, reorganization into multi-layer sheets rolled-up into tubules, and formation of a hexagonal columnar liquid crystalline phase (Jurašin et al., 2013).

Face-to-face stacking of dianionic quinoid rings in crystals

A series of alkali ($M^+ = K^+, NH_4^+, Rb^+$ and Cs^+) salts of 2,5-dihydroxyquinone [$M_2^+(C_6H_4O_4)^{2-}$] were prepared and their structures were determined by X-ray structure analysis. A less-common type of π -stacking of dianionic quinoid rings in face-to-face fashion was observed. However, in the potassium salts the stacking motif of the dianionic quinoid rings was a herring-bone pattern, usually observed in the stacking of aromatics. The different types of crystal structures, induced by various cations, are discussed in terms of the relative energies calculated by the DFT method. The energy of interaction was 6-8 kcal mol⁻¹, which is an

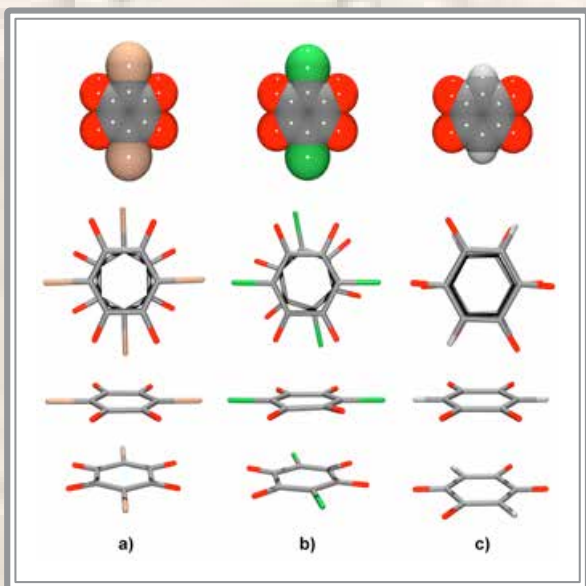


Fig 6. Pairs of contiguous quinoid rings in face-to-face stacks: (a) hydrogen bromanilate monoanions in a staggered arrangement, (b) hydrogen chloranilate monoanions in a partially staggered arrangement and (c) DHQ dianions in an eclipsed arrangement.

order of a magnitude stronger than typical aromatic π -stacking and comparable to medium-strong hydrogen bonds. The stacking of the quinoid rings is assisted by dispersion interactions (Molčanov et al., 2013).

Mechanism and kinetics of addition of OH radical to fluorobenzene

The main atmospheric degradation pathway for aromatic pollutants like fluorobenzene is initiated by a hydroxyl radical due to its high oxidation potential. All geometries and energies significant for the first step of tropospheric degradation of fluorobenzene were characterized using the MP2/6-31+G(d,p) and G3 methods. A pre-reaction complex for the addition of an OH radical to fluorobenzene was found and the associated transition state was determined for the first time. The experimental reaction rates and their unusual temperature dependence were successfully reproduced by RRKM theory coupled with the particle-in-a-box approximation in the temperature range of environmental concern. Regioselectivity, determined from the ratio of respective reaction rates is in very good agreement with experimental results, which show the dominance of *ortho* and *para* channels and a negligible contribution of the *ipso* channel (Kovačević and Sabljčić, 2013).

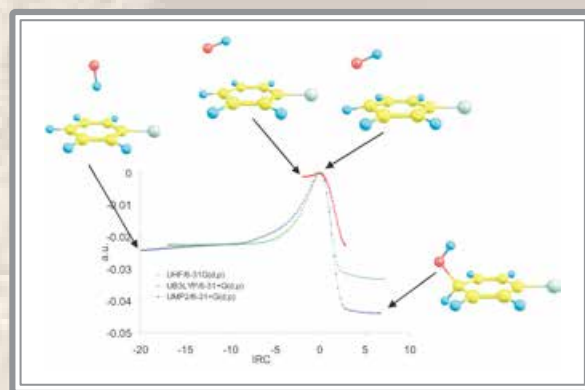


Fig 7. The detailed reaction mechanism and energy profile of OH radical addition to fluorobenzene.

ERC frontier research project - Biological membranes in action (MEMBRANESACT)

The formation and transport of supramolecular complexes in membranes is ubiquitous to nearly all functions of biological cells. Today, there is a variety of experiments suggesting that macromolecular complexes act as scaffolds for free proteins, overall yielding obstructed diffusion, counterbalanced by active transport by molecular motors. However, an integrative view connecting complexation and transport is largely missing. Furthermore, the effects of membrane mediated interactions and (non)-thermal fluctuations were so far overlooked. Gaining a quantitative insight into these processes is key to understanding the fundamental functioning of cells. In this context, the aim of this proposal is to bridge the gap between the two worlds and significantly contribute to both physics and the life sciences by developing general principles that can be applied to processes in cells. Resolving these issues is of fundamental importance since it would identify how interactions on the cell surface arise, and may translate directly into pharmaceutical applications.

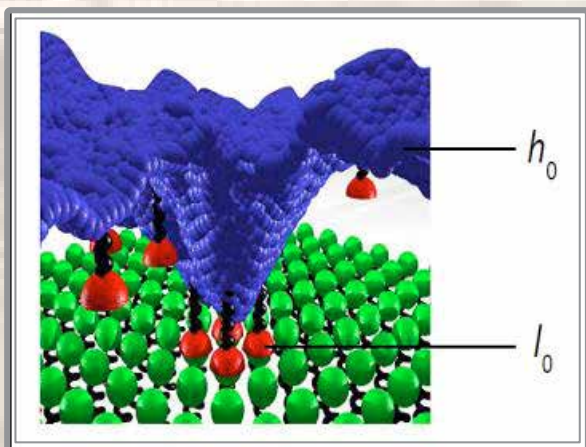


Fig 8. A schematic membrane with embedded ligands binding to a flat substrate containing specific receptors.

EDUCATION

Division members provided more than 30 undergraduate and graduate courses at Universities in Zagreb, Split, Rijeka, Osijek and Dubrovnik.

PROJECTS

Program supported by the Ministry of Science, Education and Sport

1. Molecular structure, dynamics and reactivity.
Program leader: Boris Rakvin

Projects supported by the Ministry of Science, Education and Sport

1. Molecular structure and dynamics of systems with paramagnetic particles, Boris Rakvin
2. Surfactants, processes in solutions and at interfaces, Maja Dutour Sikirić
3. Measurement and effect of atmospheric oxidants, Leo Klasinc
4. Advanced studies on chemical reactivity, Aleksandar Sabljic
5. Design, synthesis and properties of organic ligands and their metal complexes, Manda Ćurić
6. Protein-ligand interactions at atomic level, Marija Luić
7. Spectroscopy, chemical properties and reactions of biologically active molecules, Branka Kovač
8. Control of atomic and molecular dynamics by shaped electromagnetic fields, Nađa Došlić
9. Computational study of bio-macromolecules and development of new algorithms, Sanja Tomić
10. Development of mathematical methods for the description of molecular structure, dynamics and reactivity, Darko Babić
11. Amino-beta-lactams-synthrons for biologically interesting compounds, Ivan Habuš

Research, developmental and international projects

1. Biological membranes in action: A unified approach to complexation, scaffolding and active transport, A. S. Smith (ERC frontier research project)
2. Time resolved photoelectron spectroscopy as a probe for ultrafast dynamics, N. Došlić, (UKF cooperability project)
3. Multifunctional composite coatings for bone implants, M. Dutour Sikirić (BICRO project PoC4_11_3)
4. Study of plant enzymes from metallopeptidase families M20 and M49, S. Tomić, M. Abramić, B. Salopek Sondi, B.J. Ludwig-Müller, R. Wade (AvH research group linkage project)
5. The study of condensed matter by EPR: Dynamics in glassy and crystalline matrices, M. Ilakovac Kveder (AvH research group linkage project)
6. Supramolecular chemistry in water, M. Ilakovac Kveder (COST CM1005)
7. Nanospectroscopy, M. Ilakovac Kveder (COST Action MP1302)
8. Advance ESR techniques on chemistry, B. Rakvin (Bilateral project with Austria)
9. Synthesis, identification and biological activity testing of novel beta lactam cholesterol absorption inhibitors, I. Habuš (Bilateral project with Austria)
10. Correlation of structural characteristics and physical properties of quinoid rings leads to novel functional materials, K. Molčanov (Bilateral project with Slovenia)
11. Antifungal activity of novel dithiocarbamate complexes with transition metals, A. Višnjevac (Bilateral project with Montenegro)
12. Computer program for mass spectrometry data reduction collected during protein cross-linking experiments, S. Kazazić (HAZU project)

SELECTED INVITED LECTURES

1. Rakvin B. EPR study of relaxation rate of glassy modes in hydrogen bonded solid.

XXV International EPR Seminar, Častá-Papiernička, Slovak Republic, April 10–12, 2013.

2. Došlić N. Snapshots of excited state hydrogen bond dynamics. 20th International Conference on Horizons in Hydrogen Bond Research, University of Antwerp, Antwerp, Belgium, September 15-20, 2013.
3. Dutour Sikirić M. Light scattering techniques for nanoparaticles characterization. Nanobiotechnology International Workshop, Ispra, Italy, December 3-5, 2013.
4. Tomić S (2013) Chemistry Noble Prize in 2013. HAZU, Zagreb, Croatia, October 24, 2013.

SELECTED PUBLICATIONS

1. Krunoslav U, Halasz I, Đilović I, Bregović N, Rubčić M, Matković-Čalogović D, Tomišić V. Dynamic molecular recognition in solid state for separating mixtures of isomeric dicarboxylic acids. *Angew Chem Int Ed* **52** (2013) 5504.
2. Juribašić M, Budimir A, Kazazić S, Čurić M. Dicyclopalladated complexes of asymmetrically substituted azobenzenes: synthesis, kinetics and mechanisms. *Inorg Chem* **52** (2013) 12749.
3. Kovačević G, Sabljic A. Theoretical study on the mechanism and kinetics of addition of hydroxyl radicals to fluorobenzene. *J Comput Chem* **34** (2013) 646.
4. Ljubić I, Matasović B, Bonifačić M. An efficient buffer-mediated control between free radical substitution and proton-coupled electron transfer: dehalogenation of iodoethane by the α -hydroxyethyl radical in aqueous solution. *Phys Chem Chem Phys* **15** (2013) 18001.
5. Jurašin D, Vinceković M, Pustak A, Šmit I, Bujan M, Filipović-Vinceković N. Lamellar to hexagonal columnar liquid crystalline phase Transition in a catanionic surfactant mixture : dodecylammonium chloride/sodium bis(2-ethylhexyl) sulfosuccinate. *Soft Matter* **9** (2013) 3349.
6. Molčanov K, Jurić M, Kojić-Prodić B. Stacking of metal chelating rings with π -systems

- in mononuclear complexes of copper(II) with 3,6-dichloro-2,5-dihydroxy-1,4-benzoquinone (chloranilic acid) and 2,2'-bipyridine ligands. *Dalton Trans* **42** (2013) 15756.
7. Molčanov K, Kojić-Prodić B, Babić D, Stare J. Face-to-face stacking of dianionic quinoid rings in crystals of alkali salts of 2,5-dihydroxyquinone in view of π -system polarization. *Crystengcomm* **15** (2013) 135.
 8. Kovačević G, Sabljic A. Mechanisms and reaction-path dynamics of hydroxyl radical reactions with aromatic hydrocarbons: the case of chlorobenzene. *Chemosphere* **92** (2013) 851.
 9. Perić I, Merunka D, Bales BL, Perić M. Rotation of four small nitroxide probes in supercooled bulk water. *J Phys Chem Lett* **4** (2013) 508.
 10. Močibob M, Ivić N, Luić M, Weygand-Đurašević I. Adaptation of aminoacyl-tRNA synthetase catalytic core to carrier protein aminoacylation. *Structure* **21** (2013) 614.
 11. Basarić N, Došlić N, Ivković J, Wang YH, Veljković J, Mlinarić-Majerski K, Wan P. Excited state intramolecular proton transfer (ESIPT) from phenol to carbon in selected penylnaphthols and naphthylphenols. *J Org Chem* **78** (2013) 1811.
 12. Paradzik T, Ivic N, Filic Ž, Manjasetty AB, Herron P, Luić M, Vujaklija D. Structure–function relationships of two paralogous single-stranded DNA-binding proteins from *Streptomyces coelicolor*: implication of SsbB in chromosome segregation during sporulation. *Nucleic Acids Res* **41** (2013) 3659.
 13. Jokanović V, Čolović B, Dutour Sikirić M, Trajković V. A new approach to the drug release kinetics of a discrete system: SiO₂ system obtained by ultrasonic dry pyrolysis. *Ultrason Sonochem* **20** (2013) 535.
 14. Radić Stojković M, Škugor M, Tomić S, Grabar M, Smrečki V, Dudek Ł, Grolik J, Eilmes J, Piantanida I. Dibenzo-tetraaza[14]annulene–adenine conjugate recognizes complementary poly dT among ss-DNA/ss-RNA sequences. *Org Biomol Chem* **11** (2013) 4077.

Review articles

1. Tušek-Božić Lj. Aminophosphonate metal complexes of biomedical potential. *Curr Med Chem* **20** (2013) 2096.



DIVISIONAL ORGANIZATION

Head: Kata Majerski

The Division of Organic Chemistry and Biochemistry (DOCB) consists of the following laboratories:

- ⇒ Laboratory for stereoselective catalysis and biocatalysis, Zdenko Hameršak
- ⇒ Laboratory for synthetic organic chemistry, Kata Majerski
- ⇒ Laboratory for supramolecular and nucleoside chemistry, Ivo Piantanida (authorised person)
- ⇒ Laboratory for carbohydrate, peptide and glycopeptide chemistry, Lidija Varga-Defterdarović
- ⇒ Laboratory for cellular biochemistry, Marija Abramić
- ⇒ Laboratory for physical organic chemistry, Davor Margetić
- ⇒ Laboratory for molecular spectroscopy, Goran Baranović
- ⇒ Laboratory for study of interactions of biomacromolecules, Ivo Piantanida
- ⇒ Group for quantum organic chemistry, David Smith



stry and 47 scientific papers were published, primarily in high-ranking chemical journals. Amongst the broad range of topics covered, important contributions were made in areas such as: synthetic, physical organic chemistry, photochemistry and mechanochemistry; stereoselective synthesis; supramolecular chemistry, self-assembles including gels and host-guest interactions and interactions of small molecules with DNA/RNA; the chemistry of peptides and peptidomimetics; molecular spectroscopy as well as experimental and computational protein biochemistry; the structure-function relationship and catalytic mechanism of metallopeptidases and quantum organic chemistry. Members of the Division provided significant contributions to higher education by providing numerous courses at the undergraduate and doctoral levels as well as by supervising 7 Master theses and 10 PhD theses. The Division's members were also active in national and international societies and bodies and served as editors or members of several editorial boards.

The scientists from the DOCB are important team members in the implementation of the FP7-REGPOT-2012-2013-1, Grant and Agreement Number 316289 – InnoMol.

OVERVIEW OF THE DIVISION

In 2013, the members of the Division continued to maintain their established excellence in scientific research. The Division's focus was directed towards basic research in the fields of organic and bioorganic chemi-

Among the many scientists involved, I. Piantanida, I. Jerić, M. Roje, and D. Smith are the leaders of the following work packages: Equipment Implementation & Exploitation, IPR Management, Dissemination & Visibility Activities, and Management, respectively. The project budget enabled an upgrade of the equipment for chiroptical spectroscopy (CD/ORD upgraded by LD attachment) and acquisition of equipment for microcalorimetry (high sensitivity ITC and DSC). The new equipment is available not only to the InnoMol team members, but also to all scientists from DOCB and RBI. This new infrastructure will provide a higher-level working environment necessary for the enhancement of research potential.

TOP ACHIEVEMENTS

Computational design of organic superbases

New superbasic guanidines with heteroalkyl side chains, able to form intramolecular H-bonds, have been computationally designed. The resulting structures are calculated to have gas phase proton affinities (PA) between 286 and 293 kcal mol⁻¹ and pK_a values in acetonitrile between 29.5 and 33.2 (Barić et al., 2013), which makes them the most basic guanidines designed so far (Figure 1a). A more detailed analysis of various effects that may influence the PA of heteroalkyl substituted guanidines revealed that not only do intramolecular hydrogen bonds play an important role but the inductive effect of the molecular fragment at the end of alkyl chain and the alkyl chain itself also have significant influences on the PA. Two novel bisphosphazene proton sponges, 1,8-bis (trispyrrolidinophosphazene) naphthalene (TPPN) and its higher homologue P2-TPPN, have been synthesized and computationally characterized (Kögel et al., 2013). They exhibit pK_{BH}⁺ values in acetonitrile of 32.3 and 42.1, respectively, exceeding the existing basicity record for proton sponges by more than 10 orders of magni-

tude. Theoretical calculations revealed that the major contribution to the higher basicity of TPPN and P2-TPPN compared to the previously synthesized HMPN proton sponge is a higher basicity of substituents on the naphthalene backbone, whereas a contribution from the proton chelating effect is less pronounced (Kögel et al., 2013).

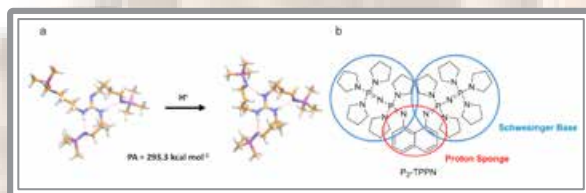


Fig. 1. Organic superbases of the guanidine (a) and bisphosphazene (b) families.

Chiral hexa- and nona-methylene bridged bis(L-Leu-oxalamide) gelators. First oxalamide gels containing aggregates with chiral morphology

Chiral dioxalamide dimethyl ester 1₆Me, 1₉Me and dicarboxylic acid 2₆OH, 2₉OH derivatives containing flexible methylene brid-

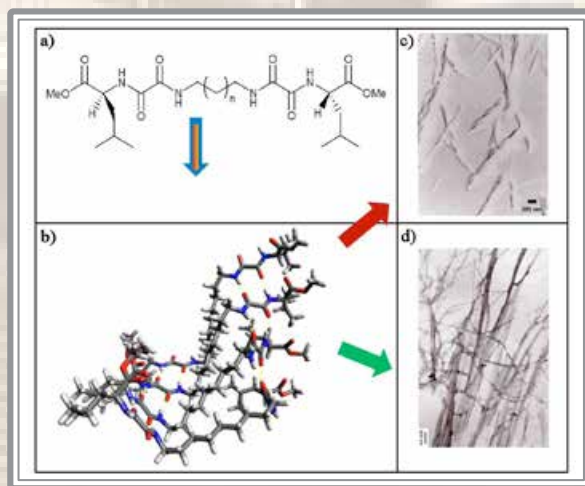


Fig. 2. a) Chiral hexa- and nona-methylene bridged bis(L-Leu-oxalamide) gelators containing flexible methylene bridges with odd (9; n = 7) and even (6; n = 4) number of methylene groups are capable of b) forming diverse chiral aggregates, c) resulting with right handed twisted ribbons (2-octanol gel; widths of 30–180 nm) and d) the simultaneous presence of aggregates of diverse morphology in the same DMSO-water gel system, the helical fibers (d's 20–40 nm) together with nano-tubule bundles (d's 40–120 nm).

ges with odd (9; $n = 7$) and even (6; $n = 4$) number of methylene groups were prepared. Their self-assembly motifs and gelation properties were studied by a number of methods (FTIR, $^1\text{H-NMR}$, CD, TEM, DSC, XRPD, molecular modelling, MMFF94 and DFT). In contrast to the previously studied chiral bis(amino acid, or amino alcohol) oxalamide gelators the conformationally more flexible 1_6Me , 1_9Me , 2_6OH and 2_9OH endow gelators capable of forming diverse aggregates of achiral and chiral morphologies such as helical fibers, twisted tapes, nano-tubules, straight fibers and tapes in some cases co-existing in the same gel sample (Šijaković Vujičić et al., 2013).

Tuning the structure-properties relationship of liquid crystals

The work described herein considers a series of novel symmetric naphthyl-based liquid crystalline dimers to show how the observed molecular organization is governed by the competition between geometrical factors and the dipole-dipole interaction between identical mesogenic units. The results present a new insight into the intermolecular forces influencing the nature of molecular packing. Understanding the factors governing the molecular arrangement within the mesophase is essential for controlling the self-organizing processes of a single functional moiety into periodically ordered nanostructures and can significantly help in the design of new soft organic materials with specific properties (Šepelj et al., 2013).

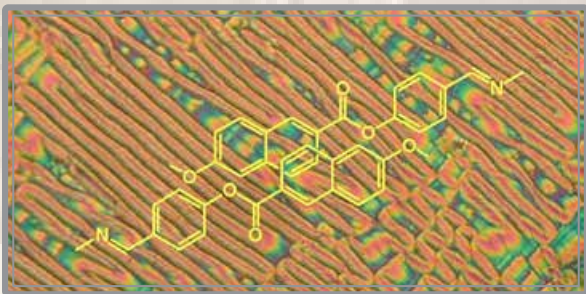


Fig. 3. Picture of the rope texture of the Nx phase.

ESIPT to carbon

Excited state intramolecular proton transfer (ESIPT) and solvent-assisted ESPT in isomeric phenyl naphthols and naphthyl phenols was investigated via preparative photolyses in $\text{CH}_3\text{CN-D}_2\text{O}$, fluorescence spectroscopy, laser flash photolyses, and *ab initio* calculations. A combination of experiments and theoretical investigations indicate that the efficiency of the ESIPT and solvent-assisted PT is mainly determined by different populations of the reactive conformers in the ground state and the NEER (non equilibration of the excited state rotamers) principle (Figure 4). ESIPT takes place *via* conical intersections of the S_1 and S_0 surfaces, whereas solvent-assisted PT takes place *via* a sequential mechanism involving first deprotonation of the phenol/naphthol, followed by the protonation by H_2O in the S_1 state of phenolate/naphtholate (Basarić et al., 2013).

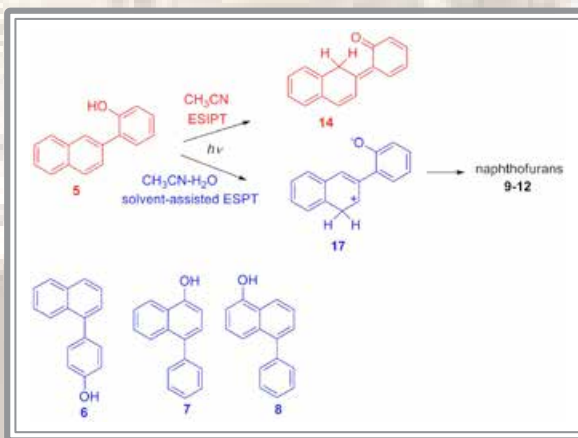


Fig. 4. Investigated molecules undergoing ESIPT or ESPT.

Photoinduced H-abstraction in constrained media

Photochemical reactivity of homo- and pro-toadamantylphthalimides was investigated in different media: solution, β -cyclodextrine complex and the solid state. It was found that complexation with β -cyclodextrine changes regiochemistry of the H-abstraction (Cindro et al., 2013).

Photodeactivation paths in norbornadiene

A new mechanism for photodeactivation of an electronically excited norbornadiene in the gas phase, was investigated by high level *ab initio* quantum-chemical calculations (MR-CIS and CASPT2). The mechanism described in this work raises some doubts in the assignment of excited states and in the interpretation of processes that are behind the experimentally obtained time constants for the ultrafast deactivation. It was shown that deactivation from the first valence excited state take place through conical intersection of the Olivucci-Robb type (Antol, 2013).

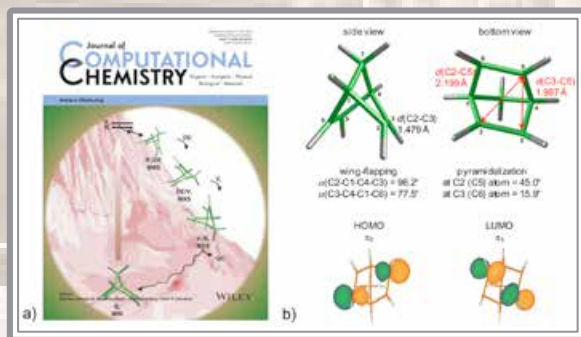


Fig. 5. a) Cover page of the *Computational Chemistry* 34/2013 depicting an artistic view on a norbornadiene "avalanche" rolling down the slopes and jumping between different potential energy surfaces toward the ground state minimum. b) The V_1/S_0 MXS asymmetrical structure of norbornadiene calculated by the MR-CIS method.

Insight into the binding between the physiological form of glutathione and cadmium dication Cd^{2+} in aqueous solution

DFT calculations were employed to investigate the nature of binding between glutathione and cadmium dication (Cd^{2+}) in water. The results revealed that, upon complexation, the cysteine $-\text{SH}$ group gets deprotonated by the neighboring glycine carboxylate, reverting the latter to its unionized form, with not enough nucleophilicity to coordinate Cd^{2+} . The process is facilitated by the formation of favourable $\text{Cd}^{2+}\backslash\text{S}^-$ coordination,

which reduces cysteine $\text{pK}_a(\text{SH})$ value by 18 pK_a units. These findings are fully consistent with vibrational and NMR spectroscopic measurements reported earlier (Glušić et al., 2013).

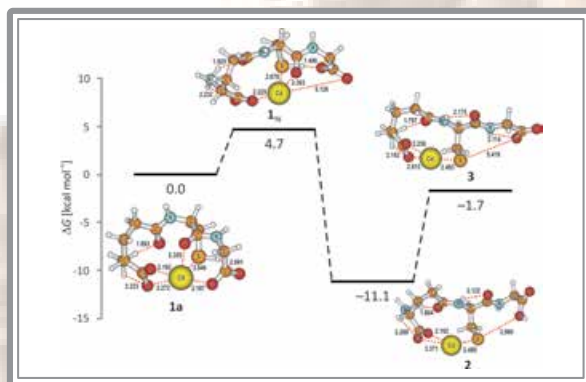


Fig. 6. Free energy profile for the deprotonation of the glutathione $-\text{SH}$ group induced upon binding to Cd^{2+} dication.

Interactions of monovalent salts with cationic lipid bilayers

It was shown by a combination of advanced experimental and computational methods that certain negatively charged ions can modify the permeability of positively charged DOTAP phospholipid bilayers. This finding can have important consequences for various medical purposes, such as further development of genetic therapy (Pokorna et al., 2013).

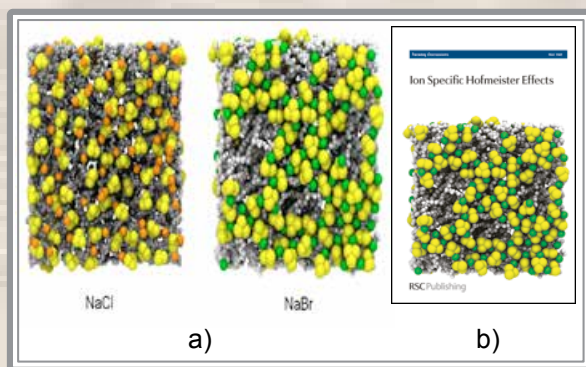


Fig. 7. a) Clustering of cationic DOTAP lipids by Br^- anions, b) Cover page of *Faraday Discussions* 160/2013 depicting clustering of cationic DOTAP lipids by Br^- anions.

Dibenzotetraaza[14]annulene – adenine conjugate recognizes complementary poly dT among ss-DNA / ss-RNA sequences

Study of various aspects of DNA/RNA recognition by small organic molecules resulted in 4 scientific publications in CC/Wos referenced journals, among which the most intriguing was a report on the first small molecule able to specifically recognize consecutive oligo dT sequence by affinity and specific chiroptical (ICD) response (Radić Stojković et al., 2013).

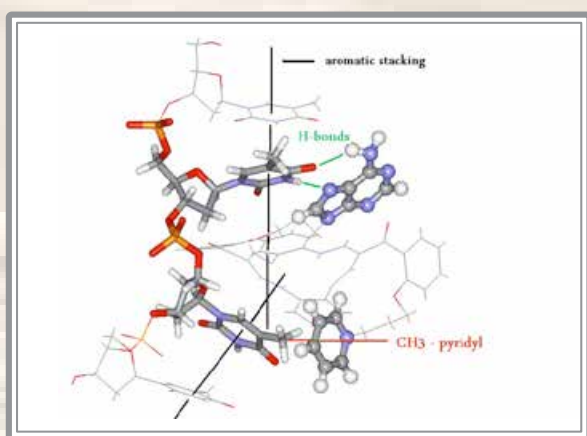


Fig. 8. Structure of a 1(stick-model)/oligo dT(line model) complex obtained by molecular modelling, which demonstrates structural parameters of recognition.

EDUCATION

Members of the Division provided significant contributions to higher education by providing numerous courses at the undergraduate and doctoral levels at the Universities of Zagreb, Rijeka, Osijek, Split, Dubrovnik and Mostar (BIH). Members of DOCB are involved in several PhD programs, in particular, Chemistry – PhD program at the Faculty of Science, University of Zagreb; Medicinal Chemistry – PhD Program at the University of Rijeka, and Chemistry of Mediterranean Environment – PhD Program at the University of Split.

AWARDS

1. Vjekoslav Štrukil received the Croatian State Award for Scientific Novices in Natural Sciences for the year 2013.
2. Matija Gredičak received a financial support for the research training at the University of Oxford, Department of Chemistry, UK, prof. Martin D. Smith, September, 2012 – August, 2013.
3. Award to Robert Vianello: Presentation of research achievements on the official web-site of the European Commission (<http://www.croatia-in-the-eu.eu>) celebrating Croatia's accession to the European Union.

PROJECTS

Programs supported by the Ministry of Science, Education and Sport

1. New small molecules targeting macromolecules of tumor and inflammatory processes, No: 0982914, Ivo Piantanida
2. Design, synthesis and reactivity of (bio)organic molecular systems, No: 0982933, Mirjana Maksić

Projects supported by the Ministry of Science, Education and Sport

1. Chiral building blocks for biological active molecules. Synthesis and reactivity, Zdenko Hameršak
2. Chiral organic materials - synthetic, structural and functional research, Vladimir Vinković
3. Cage Compounds: Building Blocks for Molecular Architecture, Kata Majerski
4. Self-assembly in gels and synthesis of functional hybrid materials, Leo Frkanec
5. Synthesis of novel biologically active nucleobase and nucleotide derivatives, Biserka Žinić
6. Chemical transformations of natural compounds, Lidija Varga-Defterdarović
7. Molecular enzymology and protein interactions of hydrolases, Marija Abramić
8. 'Host-guest' interactions in polycyclic systems, Davor Margetić

9. Organic and bioorganic processes in ground and electronically excited states, Mirjana Maksić
10. Macrocyclic ligands, structures in solutions and molecular spectroscopies, Goran Baranović
11. Design, synthesis and study of interactions of small molecules with DNA, RNA and proteins, Ivo Piantanida
12. Brönsted and Lewis acids and bases in chemistry and biochemistry, Robert Vianello.
13. Computational studies of protein structure and function, David Smith.
8. Study of plant enzymes from metallopeptidase families M20 and M49. RBI project partners: S. Tomić, M. Abramić, B. Salopek-Sondi, A. von Humboldt Foundation, institutional partnership 2012-2014.
9. Synthesis and efficacy of chlorophyllin derivatives as photosensitizers for photodynamic therapy, Davor Margetić, Croatian-Chinese Scientific and Technological Cooperation, 6-11, 2013–2015.
10. Interactions of small organic molecules with nucleic acids: Synthesis, structural features and thermodynamics, Ivo Piantanida, Bilateral project Croatia-Slovenia, 2012–2013.
11. A Combined computational chemistry and mass spectrometry approach for improved detection of endogenous metabolites in living organisms. Borislav Kovačević, Bilateral project DAAD Croatia-Germany, 2013–2014.
12. Diversity in metallopeptidase family M49, Marija Abramić, Bilateral project Croatia-Austria, 2012-2013.
13. Supramolecular Chemistry in Water, Ivo Piantanida, COST Action CM1005, 2011–2015.
14. The Network for the Biology of Zinc (Zinc-Net), Renata Kobetić, COST Action TD 1304, 2013–2017.

Research, developmental and international projects

1. “Computational Studies of the Biogenic Amines of the Brain for Targeting Neurological Diseases (CompBAND)”, Robert Vianello, Individual Marie Curie Career Integration Grant, FP7–PEOPLE–2012–CIG call, FP7–334493, 2013–2017.
2. Artificial Receptors for Bacillus anthracis Specific Anthrose Detection. Andreja Jakas and Predrag Cudic, NATO Science for Peace and Security Programme, CBP.EAP. SFP.983154., 2008–2013.
3. Enhancement of the Innovation Potential in SEE through new Molecular Solutions in Research and Development (InnoMol). Project Coordinator Oliver Vugrek, FP7-REG-POT-2012-2013-1, 2013–2016.
4. Photochemistry of polycyclic molecules: From mechanistic studies to new drugs and medicinal applications, Nikola Basarić, HRZZ 02.05/25, 2010–2013.
5. Emergence and Evolution of Complex Chemical Systems, Leo Frkanec, EU COST CMST Action CM1304, 2013–2017.
6. Optimizing bidirectional “highway” for photoactive response through guanidine-chromophore junction. Ivana Antol, Bilateral project DAAD, Croatia-Germany, 2012–2013.
7. Design and synthesis of novel chiral cationic perylene bisimides and study of their interactions with DNA/RNA, Ivo Piantanida, Bilateral project DAAD, Croatia-Germany, 2012–2013.

SELECTED INVITED LECTURES

1. Basarić N (2013) Quinone methides: photochemical generation and antiproliferative activity. XXIII Croatian Meeting of Chemists and Chemical Engineers, Osijek, Croatia, April 21-24, 2013.
2. Vianello R (2013) How are biogenic amines metabolized by monoamine oxidases? Summer School: From Computational Enzymology towards Molecular Docking, University of Ljubljana, Slovenia, May 31, 2013.
3. Vianello R (2013) Computational insight into the catalytic activity and irreversible inhibition of monoamine oxidase for targeting neurological diseases. 12th National Conference on Biophysics “CNB 2013”, Iasi, Romania, June 13–16, 2013.

4. Vazdar M (2013) Molecular dynamics simulations - The application in biologically relevant processes. University of Veterinary Medicine, Vienna, Austria, July 3, 2013.
5. Basarić N (2013) Quinone methides in the photodehydration of 2-hydroxy-3-hydroxy-methyl)anthracenes. International Conference on Photochemistry, Leuven, Belgium, July 21-26, 2013.
6. Eckert-Maksić M (2013) Search for strong guanidine bases. Theory and experiment in concert. The 14th European Symposium on Organic Reactivity, Prague, Czech Republic, September 1-6, 2013.
7. Vianello R (2013) Recent progress in understanding the catalytic activity of monoamine oxidases. Interdisciplinary Chemical Approaches for Neuropathology, Valletta, Malta, October 22–25, 2013.
- Bisphosphazene Proton Sponges: The Run for the Best Chelating Ligand for a Proton. *J Am Chem Soc* **35** (2013) 17768.
3. Šijaković Vujičić N, Glasovac Z, Zweep N, van Esch JH, Vinković M, Popović J, Žinić M. Chiral hexa- and nona-methylene bridged bis(L-Leu-oxalamide) gelators. First oxalamide gels containing aggregates with chiral morphology. *Chem Eur J* **19** (2013) 8558.
4. Džolić Z, Cameti M, Milić D, Žinić M. The Formation of CuCl₂-Specific Metallogels of Pyridyloxalamide Derivatives in Alcohols. *Chem Eur J* **19** (2013) 5411.
5. Horvat G, Stilinović V, Kaitner B, Frkanec L, Tomišić V. The Effect of Specific Solvent-Solute Interactions on Complexation of Alkali-Metal Cations by a Lower-Rim Calix[4]arene Amide Derivative. *Inorg Chem* **52** (2013) 12702.
6. Basarić N, Došlić N, Ivković J, Wang Y-H, Veljković J, Mlinarić-Majerski K, Wan P. Excited State Intramolecular Proton Transfer (ESIPT) from Phenol to Carbon in Selected Phenylanthracenes and Naphthylphenols. *J Org Chem* **78** (2013) 1811.
7. Barić D, Dragičević I, Kovačević B. Design of Superbasic Guanidines: The Role of Multiple Intramolecular Hydrogen Bonds. *J Org Chem* **78** (2013) 4075.
8. Antol I. Photodeactivation paths in norbornadiene. *J Comput Chem* **34** (2013) 1439.
9. Pokorna S, Jurkiewicz P, Cwiklik L, Vazdar M, Hof M. Interactions of monovalent salts with cationic lipid bilayers. *Faraday Discuss* **160** (2013) 341.
10. Vazdar M, Jungwirth P, Mason P. Aqueous Guanidinium-Carbonate Interactions by Molecular Dynamics and Neutron Scattering: Relevance to Ion-Protein Interactions. *J Phys Chem B* **117** (2013) 1844.
11. Šepelj M, Baumeister U, Ivšić T, Lesac A. Effects of Geometry and Electronic Structure on the Molecular Self-Assembly of Naphthyl-Based Dimers. *J Phys Chem B* **117** (2013) 8918.
12. Radić Stojković M, Škugor M, Tomić S, Grabar M, Smrečki V, Dudek Ł, Grolik J, Eilmes J, Piantanida I. Dibenzotetraaza[14]

SELECTED PLENARY LECTURE

1. Piantanida I. Sensing the shape of the ds-DNA/RNA structures by non-covalent interactions. 23rd Croatian Meeting of Chemists and Chemical Engineers, Osijek, HR, April 21–24, 2013.
2. Vianello R. Computational analysis of the catalytic activity and irreversible inhibition of monoamine oxidase for targeting neurological diseases. 6th Central European Conference – Chemistry towards Biology, Trieste, Italy, September 10–13, 2013.)

SELECTED PUBLICATIONS

1. Halasz I, Puškarić A, Kimber SAJ, Beldon PJ, Belenguer AM, Adams F, Honkimki V, Dinnebier RE, Patel B, Jones W, Štrukil V, Friščić T. Real-Time In Situ Powder X-ray Diffraction Monitoring of Mechanochemical Synthesis of Pharmaceutical Cocrystals. *Angew Chem Int Ed* **52** (2013) 11538.
2. Kögel JF, Oelkers B, Kovačević B, Sundermeyer JA. New Synthetic Pathway to the Second and Third Generation of Superbasic

- annulene–adenine conjugate recognizes complementary poly dT among ss-DNA/ss-RNA sequences. *Org Biomol Chem* **11** (2013) 4077.
13. González-García J, Uzelac L, Kralj M, Llinares JM, García-España E, Piantanida I. The size of aryl linker between two polyaza-cyclophane moieties controls the binding selectivity to ds-RNA vs ds-DNA. *Org Biomol Chem* **11** (2013) 2154.
 14. Cindro N, Halasz I, Mlinarić-Majerski K, Basarić N. Photoinduced H-abstraction in homo- and protoadamantylphthalimide derivatives in solution and in organized and constrained media. *Eur J Org Chem* (2013) 929.
 15. Glušić M, Stare J, Grdadolnik J, Vianello R. Binding of cadmium dication to glutathione facilitates cysteine –SH deprotonation: a computational DFT study. *J Inorg Biochem* **119** (2013) 90.
 16. Matković M, Vukelić S, Cirimotić R, Kragol G, Molčanov K, Mlinarić-Majerski K. Synthesis of novel adamantyl and homoadamantyl substituted β -hydroxybutyric acids. *Mol Diversity* **17** (2013) 817.

CHAPTERS IN BOOKS

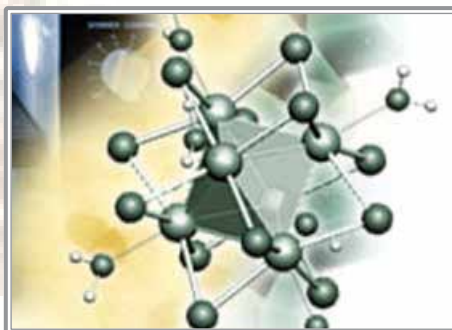
1. Jakas A (2013) Peptide Modification to Increase Metabolic Stability and Activity. Chapter 9: The Maillard reaction induced modifications of endogenous opioid peptide enkephalin, Cudic P (Ed). New York, Springer Science and Business Media, pp 137-149.
2. Piantanida I (2013) Supramolecular systems in biomedical fields. Chapter 8: Nucleic acids as supramolecular targets, Schneider H-J (Ed.). London : Royal Society of Chemistry, pp 213-259.

DIVISIONAL ORGANISATION

Head: Damir Kralj

The Division of Materials Chemistry (ZKM) consists of the following laboratories:

- ⇒ Laboratory for synthesis of new materials, Marijan Gotić
- ⇒ Laboratory for precipitation processes, Damir Kralj
- ⇒ Laboratory for radiation chemistry and dosimetry, Branka Mihaljević
- ⇒ Laboratory for solid state and complex compounds chemistry, Antun Drašner
- ⇒ Laboratory for ichthyopathology – biological materials, Rozelindra Čož-Rakovac



in various systems and materials, as well as chemical dosimetry systems. Research in the fields of ecophysiology, pathology and ecotoxicology were performed using aquatic animals as model organisms and focused on the development of new biomarkers and gene or protein expression in non-target organisms as an important response to environmental pollution.

Members of the Division participated in educational programs at the Universities of Zagreb, Osijek, Dubrovnik and Rijeka, conducting 18 undergraduate and postgraduate courses.

OVERVIEW OF THE DIVISION

The mission of the scientist of the Division of Materials Chemistry is to conduct basic and applied research on the synthesis, characterization and application of different classes of inorganic materials, such as metal oxides, glass-ceramics, silicates, slightly soluble ionic salts, cluster compounds, intermetallic compounds, metal hydrides or organic-inorganic composites. Research on polymer materials modified by fillers, polymers, and/or by ionizing radiation is primarily focused on interactions and structure-property relationships. In addition, the scientists in the Division study the physico-chemical effects and interactions of ionizing radiation

TOP ACHIEVEMENTS

A novel route in the synthesis of cubic CdS nanoparticles

A novel and simple method for the synthesis of small (2-3 nm) nanocrystallites of cubic CdS was reported. The synthesis is based on the reaction of H_2S gas with a 10% aqueous solution of $\text{Cd}(\text{CH}_3\text{COO})_2$ at room temperature: Nanosize CdS is an important material for advanced applications in photovoltaic cells as well as fabrication of thin-film transistors, diodes and phosphors (Ristić et al., 2013).

The high impact of a milling atmosphere on steel contamination

The mechanism of interaction between a milled sample and the steel milling assembly during standard high-energy ball-milling in more and lesser oxidative atmospheres was clarified. A dramatic increase in the amount of contamination during milling in a nitrogen atmosphere results from the abrasive action of steel chips that have entered into the sample due to the wear of milling tools. The amount of contamination appeared to be more than three times smaller after milling in air because small steel chips quickly oxidize and disappear in the presence of oxygen. The obtained Fe and Cr ions could easily be incorporated into the structure of a milled sample and cause significant changes in the final product (Štefanić et al., 2013).



Fig. 1. Front cover picture of the article: G. Štefanić, S. Krehula, I. Štefanić, *Chem Commun* 49 (2013) 9245-9247.

Structural and hydrogen absorption properties of $\text{SmNi}_{5-x}\text{Ga}_x$ system – an experimental and theoretical study

A series of ternary alloys having the general formula $\text{SmNi}_{5-x}\text{Ga}_x$ ($x = 0.25, 0.5, 1.5$,

2, 2.5) were prepared and hydrogen absorption ability and thermodynamic quantities were determined by pressure-composition desorption isotherms. The obtained properties were compared with those of previously reported SmNi_5 and SmNi_4Ga . DFT calculations were performed for selected members of the system and the results are discussed with regard to experiment (Biliškov et al., 2013).

A direct molecular precursor-to-material conversion

The oxalate-based compounds $\{\text{Ba}_2(\text{H}_2\text{O})_5[\text{MO}(\text{C}_2\text{O}_4)_3]\text{HC}_2\text{O}_4\} \cdot \text{H}_2\text{O}$ ($\text{M} = \text{Nb}, \text{Ta}$) were used as single-source precursors for the formation of mixed-metal oxide phases, $\delta\text{-Ba}_4\text{Nb}_2\text{O}_9$ and $\gamma\text{-Ba}_4\text{Ta}_2\text{O}_9$. These 6H-perovskite structures (space group $P6_3/m$) have interesting electrical and optical properties (Androš et al., 2013a; 2013b).

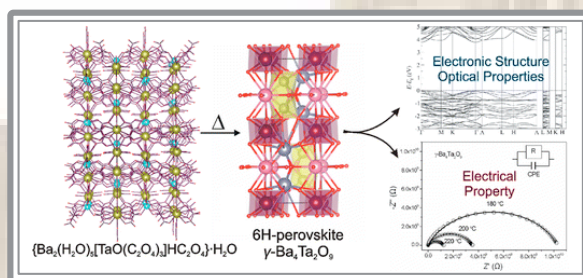


Fig. 2. Thermal treatment of $\{\text{Ba}_2(\text{H}_2\text{O})_5[\text{TaO}(\text{C}_2\text{O}_4)_3]\text{HC}_2\text{O}_4\} \cdot \text{H}_2\text{O}$ leading to 6H-perovskite polymorph of $\gamma\text{-Ba}_4\text{Ta}_2\text{O}_9$.

Artificial metalloenzymes as suitable enantioselective catalysts

Disubstituted conjugates of 5-(di-phenylphosphino)isophthalic acid with amino acids, peptides or amines were used as monodentate ligands in rhodium(I) catalyzed hydrogenation of 2-acetamidoacrylate or (Z)-(alpha)-acetamidocinnamate. By using the principle of “backdoor induction” of chirality from hydrogen-bonded amino acids to prochiral $\text{Rh}(\text{I})$, a selectivity of up to 84 % ee was obtained (Kokan and Kirin, 2013).

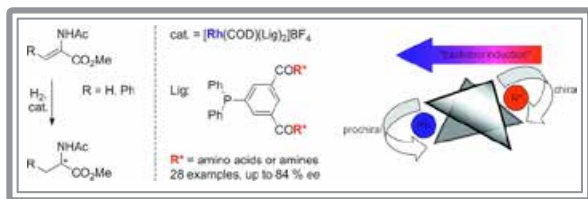


Fig. 3. Models of artificial metalloenzymes where chirality of distant hydrogen-bonded amino acids is transmitted to prochiral Rh(I) center.

Effects of a propolis enriched diet on growth performance and plasma biochemical parameters of juvenile European sea bass (*Dicentrarchus labrax* L.) under acute low temperature stress.

In order to study the effect of a water propolis extract (WEP) on *Dicentrarchus labrax* under low temperature stress, sea bass juveniles were fed a basal diet supplemented with 1.25 and 2.5 g kg⁻¹ of water propolis extract. The results of the study suggest that ingestion of a basal diet supplemented with 2.5 g kg⁻¹ of propolis extract could prevent the adverse effects of low temperature stress and promote the growth of sea bass.

The study of possible synergism of γ -irradiation and nanoparticle addition

The addition of surface modified nano-silica fillers significantly influenced the spherulitic morphology of an isotactic polypropylene (iPP) matrix but not its phase characteristics. Due to better compatibility with iPP, nonpolar nano-silica particles enhanced spherulitic growth more than polar ones. On the other hand, by increasing the content of a more radiation sensitive amorphous phase in irradiated poly(ethylene oxide)-nanocomposite films, unmodified nano-silica enhanced oxidative degradation resulting in a crystallinity increase while radiation-crosslinked nanocomposite gels had much lower crystallinity, phase transformation temperatures and better mechanical properties indicating possible synergism of γ -irradiation and nanoparticle addition.

Upgrading of irradiation facility

Long-term research in basic and applied radiation and polymer chemistry, radiation processing, radiation microbiology and radiation dosimetry led to successful funding of a technical cooperation project from the IAEA for upgrading of the ⁶⁰Co panoramic facility in the amount of 221,200-€. Upgrading of the ⁶⁰Co panoramic facility will lead to enhanced scientific and applied research in various aspects of irradiation technologies as well as quality improvement of radiation processing services and facility operation in compliance with the demands of EU legislation.

NEW EQUIPMENT

- -80°C freezer
- Fluorescence microscope
- Thermo oven

EDUCATION

In 2013, scientists and researchers from the Division contributed to educational programs at the Universities in Zagreb, Osijek, Dubrovnik and Rijeka, conducting 18 undergraduate and postgraduate courses. Division scientists actively participated in various bachelor's, master's and doctoral courses.

PROJECTS

Projects supported by the Ministry of Science, Education and Sport

1. Physico-chemical effects of ionizing radiation in materials, Branka Mihaljević
2. Structure-property relationships of modified polymer materials, Ivan Šmit
3. Synthesis and microstructure of metal oxides and oxide glasses, principal investigator, Mira Ristić
4. Study of influence of aluminosilicate precursor on their transformations, Josip Bronić
5. Metal hydrides in clean energy systems, Antun Drašner

6. Polynuclear metal systems: synthesis and properties, Berislav Perić
7. Subcellular biochemical and phylogenetic diversity of aquatic organisms, Rozelindra Čož-Rakovac
8. Precipitation mechanism of inorganic bio-compatible and related materials, Damir Kralj
9. Functional analysis and molecular characterization of wine yeasts, Sandi Orlić

Projects supported by the Croatian Science Foundation

1. Biodiversity and biotechnology characterization of bacteria from the Adriatic Sea, Sandi Orlić

Research, developmental and international projects

1. COST Action CM1201: Biomimetic Radical Chemistry, WG3 WG 3: Membrane Stress, signalling and Defences (Mihaljević B, Tartaro Bujak I)
2. STSM within COST1201: Radical Scavenging activity of resveratrol with thiyl radicals. October 14-25, 2013. (Džeba I)
3. EURADOS, WG 12: European Medical ALARA Network (EMAN), WG 9: Radiation Protection Dosimetry in Medicine, WG 3: Environmental radiation monitoring., WG 6: Computational dosimetry (Knežević Ž, Majer M, Miljanić S, Komor Ranogajec M)
4. Japan-Croatian Agreement of Collaborative Research, Chiyoda Technol. Corporation & Ruđer Bošković Institute (Knežević Ž)
5. Introducing and Harmonizing Standardized Quality Control Procedures for Radiation Technologies. IAEA Regional Technical Cooperation Project RER 1/011 (Miljanić S)
6. Enhancing the characterization, preservation and protection of cultural heritage artefacts. IAEA RER/0/034 (Pucić I, Jurkin T, Mihaljević B)
7. Investigations of factors influencing the properties of metallic and metal oxide nanoparticles; Mira Ristić, Croatian-Austrian Scientific Cooperation Programme (2012-2013)
8. Nanoparticle cell interactions: Molecular

- signaling events induced by synthesized new nanomaterials, Marijan Gotić, Croatian-German Scientific Cooperation Programme (2012-2013)
9. Ultra small metal oxide semiconductor nanoparticles for energy storage: synthesis and advanced characterization, Goran Štefanić, Croatian-German Scientific Cooperation Programme (2013-2014)
10. "Zeosorb" commercial project, Josip Bronić
11. The synthesis of metal-organic framework materials for gasses storage and separation, Josip Bronić, Croatian-Slovenian bilateral scientific cooperation project (2012-2013)
12. Functional metal complexes that bind to biomolecules, Srećko Kirin, COST Action CM1105
13. Preparation and properties of dielectric ceramics based on the mixed oxides of barium(II) and niobium(V) or tantalum(V), Marijana Jurić, Foundation of the Croatian Academy of Sciences and Arts, 1152Z02
14. Enhancement of fish production via probiotic administration, in function of enhancing competitiveness (Ministry of Agriculture), Rozelindra Čož-Rakovac
15. State of the environment and nature in the waters of Pula (Herculanea), Sandi Orlić
16. Microbial ecology & earth system: collaborating for insight and success with the new generation of sequencing systems (COST action), Sandi Orlić
17. Cyanobacterial blooms and toxins in water resources: Occurrence, impacts and management (COST action), Sandi Orlić
18. System biocatalysis (COST action), Sandi Orlić

SELECTED INVITED LECTURES

1. Džeba I, Pedzinski T, Mihaljević B (2013) Photophysical and photochemical properties of resveratrol. The 28th Miller Conference on Radiation Chemistry. Dead Sea, Israel, March 14-19, 2013.
2. Tartaro Bujak I, Mihaljević B, Chatgililoglu C (2013) A biomimetic model of free radi-

- cal reactivity: The influence of antioxidants in the thiyl radical induced lipid peroxidation and isomerization processes. The 28th Miller Conference on Radiation Chemistry Dead Sea, Israel, March 14-19, 2013.
3. Knežević Ž, Trianni A, Farah J, Carinou E, Clairand I, Dabin J, De Angelis C, Domienik J, Järvinen H, Kopec R, Majer M, Malchair F, Negri A, Novák L, Siiskonen T, Vanhavere F (2013) Trigger levels for patient skin doses in interventional radiology- Overview of activity within EURADOS WG12 (SG2). The 9th International Workshop on Ionizing Radiation Monitoring (IWIRM) Oarai, Japan, November 30 - December 1, 2013.
 4. Miljanić S (2013) Glass rod dosimeter in patient dosimetry- an overview. The 9th International Workshop on Ionizing Radiation Monitoring (IWIRM) Oarai, Japan, November 30 - December 1, 2013.
 5. Miljanić S (on behalf of EURADOS WG 9) (2013) Out of field dose measurement in radiotherapy – Activity of EURADOS WG9: Radiation Protection in Medicine. 17th International conferences on solid state dosimetry (SSD17), Recife, Brazil, September 22-27, 2013.
 6. Subotić B (2013) The role sub-colloidal (nano-sized) precursor species in zeolite crystallization. 5th Serbian-Croatian-Slovenian Symposium on Zeolites, Zlatibor, Serbia, May 31-June 2, 2013.
 7. Strunjak-Perović I (2013) The use of probiotics in aquaculture. 10th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, June 28, 2013.

SELECTED ORGANIZED CONFERENCES

1. 9th Symposium of the Croatian Radiation Protection Association with International Participation, Krk, Croatia, April 10-12, 2013 (Knežević Ž and Majer M)
2. Meeting of WG 3 within COST 1201: Biomimetic Radical Chemistry, Zadar, Croatia, September 11-12, 2013. (Tartaro Bujak I and Mihaljević B)

3. Enhancing the Characterization, Preservation and Protection of Cultural Heritage Artefacts. IAEA RER 0/034 2012-2013: - Training Course on Dating of Cultural Heritage Artefacts using Nuclear Analytical Techniques, Zagreb, May 20-24, 2013 (Pucić I, Jurkin T, Mihaljević B).
4. International Conference on the Applications of the Mössbauer Effect, ICAME-2013, Opatija, Croatia, September 1-6, 2013 (Musić S and Ristić M)
5. Coorganizers of the 5th Serbian-Croatian-Slovenian Symposium on Zeolites, Zlatibor, May 31-June 2, 2013. (Bronić J, Subotić B).

SELECTED PUBLICATIONS

1. Halasz I, Puškarić A, Kimber S A J, Beldon P J, Belenguer A M, Adams F, Honkimäki V, Dinnebier R E, Patel B, Jones W, Štrukil V, Friščić T. Real-Time In Situ Powder X-ray Diffraction Monitoring of Mechanochemical Synthesis of Pharmaceutical Cocrystals. *Angew Chem Int Ed* **52** (2013) 11538.
2. Ristić M, Popović S, Ivanda M, Musić S. A simple route in the synthesis of CdS nanoparticles. *Mat Lett* **109** (2013) 179.
3. Štefanić G, Krehula S, Štefanić I. The high impact of a milling atmosphere on steel contamination. *Chem Commun* **49** (2013) 9245.
4. Palčić A, Subotić B, Valtchev V, Bronić J. Nucleation and crystal growth of zeolite A synthesised from hydrogels of different density. *Cryst Eng Comm* **15** (2013) 5784.
5. Ren N, Bronić J, Bosnar S, Dutour Sikirić M, Antonić Jelić T, Mao J-J, Subotić B. The relationship between sub-micrometer sized ZSM-5, slice-like (lamellar) keatite and hollow α -quartz particles: A phase transformation study. *Cryst Eng Comm* **15** (2013) 5032.
6. Biliškov N, Miletić GI, Drašner A. Structural and hydrogen sorption properties of $\text{SmNi}_{5-x}\text{Ga}_x$ system – an experimental and theoretical study. *Int J Hydrogen Energy* **38** (2013) 12213.
7. Maghrbi Y, Gregor R, Knežević A, (MAMI, TAPS, A2 Collaboration, Double pion photoproduction off nuclei - Are there effects be-

yond final-state interaction? *Phys Lett B* **722** (2013) 69.

8. Maghrbi Y, Krusche B, Knežević A, (MAMI, TAPS, A2 Collaboration). Coherent photoproduction of π^0 and eta mesons off ^7Li . *Eur Phys J A: hadrons and nuclei* **49** (2013) 38.
9. Popović J, Vrankić M, Jurić M. Tuning the Microstructure of $\gamma\text{-Ba}_4\text{Nb}_2\text{O}_9$ Polymorph Prepared from Single-Molecular Precursor. *Cryst Growth Des* **13** (2013) 2161.
10. Molčanov K, Jurić M, Kojić-Prodić B. Stacking of metal chelating rings with π -systems in mononuclear complexes of copper(II) with 3, 6-dichloro-2, 5-dihydroxy-1, 4-benzoquinone (chloranilic acid) and 2, 2'-bipyridine ligands. *Dalton Trans* **42** (2013) 15756.
11. Kokan Z, Kirin SI. "Backdoor induction" of chirality in asymmetric hydrogenation with rhodium(I) complexes of amino acid substituted triphenylphosphane ligands. *Eur J Org Chem* **36** (2013) 8154.
12. Jurić M, Popović J, Šantić A, Molčanov K, Brničević N, Planinić P. Single-Step Preparation of the Mixed Ball-NbV Oxides from a Heteropolynuclear Oxalate Complex. *Inorg Chem* **52** (2013) 1832.
13. Androš L, Matković-Čalogović D, Planinić P. A series of compounds containing various (oxalato)tantalate(V) complex anions – synthesis, properties and the mixed-metal oxide formation via thermal decomposition. *Cryst Eng Comm* **15** (2013a) 533.
14. Androš L, Jurić M, Popović J, Šantić A, Lazić P, Benčina M, Valant M, Brničević N, Planinić P. $\text{Ba}_4\text{Ta}_2\text{O}_9$ Oxide Prepared from an Oxalate-Based Molecular Precursor—Characterization and Properties. *Inorg Chem* **52** (2013b) 14299.
15. Orlić S, Najdek M, Supić N, Ivančić I, Fuks D, Blažina M, Šilović T, Paliaga P, Godrijan J, Marić D. Structure and variability of microbial community a transect crossing a double gyre structure (north – eastern Adriatic Sea). *Aquat Microb Ecol* **69** (2013) 193.

CHAPTERS IN BOOKS

1. Pucić I (2013) Electrical conductivity method for in-situ monitoring of radiation reactions Radiation Synthesis of Materials and Compounds. Kharisov Boris Ildusovich, Kharisova Oxana Vasilievna, Mendez Ubaldo Ortiz (eds). Boca Raton, Florida, CRC Press, Taylor & Francis Books Inc., pp 333-344.
2. Čipak Gašparović A, Jaganjac M, Mihaljević B, Borović Šunjic S, Žarković N (2013) Assays for the measurement of lipid peroxidation. Cell senescence. Galluzzi L, Vitale I, Kepp O, Kroemer G (eds). New York: Springer Science, pp 283-297.
3. Gotić M, Jurkin T, Dražić G (2013) Hematite Nanotubes and Nanorings. Hematite Sources, Properties and Applications. Morel D (ed). New York: Nova Science Publishers, Inc., pp 85-108.
4. Musić S, Ristić M, Krehula S (2013) ^{57}Fe Mössbauer Spectroscopy in the Investigation of the Precipitation of Iron Oxides in the book *Mössbauer Spectroscopy: Applications in Chemistry, Biology, Industry, and Nanotechnology*, Sharma VK, Klingelhofer G, Nishida T (eds). John Wiley & Sons, pp 470-504.
5. Klobučar G, Štambuk A, Sauerborn Klobučar R (2013) Biološke analize utjecaja onečišćenja na okoliš. In: *Analitika okoliša (Environmental Analytics)*, Kaštelan-Macan M, Petrović M (eds), HINUS, Fakultet kemijskog inženjerstva i tehnologije, Zagreb, pp 305-338.

BOOKS

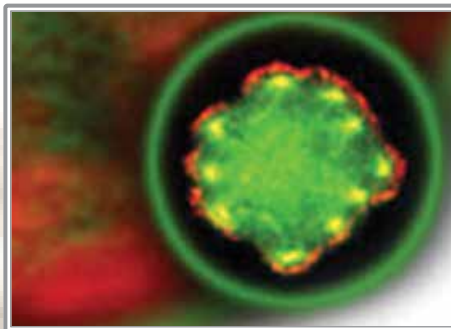
1. Proceedings of the Ninth Symposium of the Croatian Radiation Protection Association, Knežević Ž, Majer M, Krajcar Bronić I (eds), Zagreb, Croatia, HDZZ, 2013.
2. Book of the abstracts of the International Conference on the Applications of the Mössbauer Effect, ICAME-2013, Musić S, Ristić M, Krehula S, Petrović Ž (eds), Opatija, Croatia, 2013.

DIVISIONAL ORGANISATION

Head: Igor Weber

The Division of Molecular Biology consists of the following laboratories:

- ⇒ Laboratory of Neurochemistry and Molecular Neurobiology, Lipa Čičin-Šain
- ⇒ Laboratory for Electron Microscopy, Hrvoje Fulgosi
- ⇒ Laboratory for Genotoxic Agents, Maja Osmak
- ⇒ Laboratory for Structure and Function of Heterochromatin, Miroslav Plohl
- ⇒ Laboratory of Molecular and Cell Biology, Ivica Rubelj
- ⇒ Laboratory of Chemical Biology, Branka Salopek Sondi
- ⇒ Laboratory for Evolutionary Genetics, Đurđica Ugarković
- ⇒ Laboratory for Molecular Genetics, Dušica Vujaklija
- ⇒ Laboratory of Molecular Microbiology, Davor Zahradka



OVERVIEW OF THE DIVISION

The mission of the Division of Molecular Biology is to advance our knowledge on fundamental biological questions by conducting high-quality, internationally recognized knowledge-driven scientific research on major topics in contemporary biology, from molecules to cells and organisms. We also participate in knowledge transfer by contributing to education, and by offering expertise and

application of acquired knowledge, methodologies and skills to the broader community. Research areas in the Division are focused on exploring different aspects of molecular and cellular biology studied on microbial, animal and plant organisms. Particular goals of the research program are to explore non-coding repetitive sequences in genome structuring; to study structures and processes at telomeres; to study processes essential for maintaining genome integrity, plasticity and evolution; to decipher evolutionary patterns of conserved genes and appearance of new genes; to characterize general and specific transcription factors and their mechanisms of action; to study how cells communicate, differentiate, move and adhere; to investigate molecular mechanisms involved in cell response to genotoxic compounds; to examine the potential of genetically targeted adenoviruses; to explore photosynthesis; and to study the role of bioactive molecules, plant hormones and secondary metabolites, in plant growth, development and stress response.

TOP ACHIEVEMENTS

Tandem repeats as components of mobile DNA elements

A highly abundant miniature inverted-repeat transposable element (MITE) is described in the clam *Donax trunculus*. It has a complex modular structure with a short array of up to five tandemly repeated DNA segments in its central part. These repeats evolve as individual units within the MITE, while flanking sequences represent a “cassette”. Our results signify the role of transposition in the onset and initial spread of tandem repeats (Šatović and Plohl, 2013).

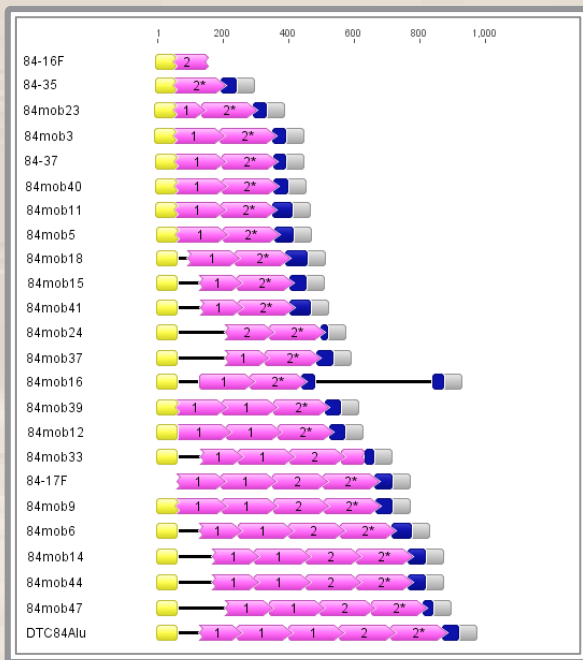


Fig. 1. Complex modular structure of the tandem repeat-containing MITE element.

Structure-function relationships of single-stranded DNA binding proteins from *Streptomyces coelicolor*

We have found a new and unexpected role of paralogous SSB protein in chromosomal segregation during the reproductive stage of multicellular bacteria that exhibit a complex

developmental program and morphological differentiation. We also report the 3D structure of SsbB with a unique interconnection by two S-S bridges between the A/B and C/D subunits. This is the first example of crystal structures of two paralogous SSB proteins from the same organism (Paradzik et al., 2013).

Transcription factor evolution

Independent transitions to multicellularity in eukaryotes involve the evolution of complex transcriptional regulation toolkits to control cell differentiation. By using comparative genomics, we show that plants and animals require richer transcriptional machineries compared with other eukaryotic multicellular lineages. Moreover, analysis of transcription factor (TF) expression patterns during the development of animals reveal links between TF evolution, species ontogeny, and the phylotypic stage (de Mendoza et al., 2013).

DNA methylation in the insect *Tribolium castaneum*

DNA methylation is implicated in developmental and phenotypic variations in many eukaryotes but, until now, no evidence of DNA methylation had been found in the red flour beetle, *Tribolium castaneum*. We report the detection of cytosine methylation in *T. castaneum* followed by global demethylation in larvae, pupae and adults. DNA methylation is preserved within heterochromatin during development and is strongly affected by heat stress, suggesting a role for DNA methylation in heterochromatin structure modulation during heat stress response (Felicciello et al., 2013).

Mechanisms of satellite DNA array rearrangements

Comprehensive analysis of six satellite DNAs, common for recently separated root-knot nematode species, suggests involvement of conserved domains in array

rearrangements and the onset of new sequence combinations. Proposed mechanisms act on short-segment tracts and indicate a highly recombinogenic nature of satellite DNA arrays (Meštrović et al., 2013).

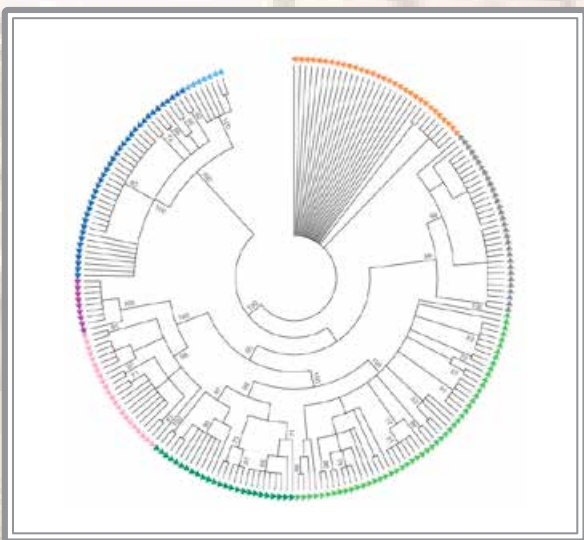


Fig. 2. The phylogenetic tree of 212 monomers extracted from higher-order repeats (H), dimeric (D) and monomeric satellite arrays (M).

Evolutionary history of relict *Congeria* (Bivalvia: Dreissenidae): unearthing the subterranean biodiversity of the Dinaric Karst

We have shown that cave bivalves are comprised of 3 allopatric lineages that descended from a last common ancestor 5.5 mya, exactly when all other *Congeria* species vanished from the fossil record. Bivalves are characterised by both morphological stasis and phenotypic plasticity but differences in the hinge plate anatomy enabled the description of two new species, separated for 2.5 my (Bilandžija et al., 2013).

EDUCATION

In 2013, members of the Division of molecular biology participated in the teaching of more than 15 undergraduate and graduate courses and more than 20 postgraduate at

the Universities in Zagreb, Split, Dubrovnik and Osijek. In 2013 they also supervised more than 15 diploma, MSc, and PhD theses.

PROJECTS

Program supported by the Ministry of Science, Education and Sport

1. Molecular fundamentals of biological processes, Miroslav Plohl.



Fig. 3. *Congeria* is the only bivalve that inhabits cave habitats. The picture shows *Congeria kusceri* that lives in south Dalmatia and Herzegovina.

Projects supported by the Ministry of Science, Education and Sport

1. Increase of adenovirus transduction efficacy and resistance to cytostatics, Andreja Ambriović Ristov
2. Molecular interactions in lymphocyte differentiation, Mariastefania Antica
3. The role of recombination in DNA repair and genome evolution, Krunoslav Brčić-Kostić
4. Genes and genomes: structure, function and evolution, Helena Četković
5. Serotonergic mechanisms in alcoholism, Lipa Čičin-Šain
6. Genetic studies of BPC-157 effect on micro-organisms, Senka Džidić
7. Regulatory mechanisms of photosynthesis and differentiation of plastids, Hrvoje Fulgosi
8. Hydrodynamics of cerebrospinal fluid, Darko Orešković

9. Cell response to cytotoxic agents and resistance development, Maja Osmak
10. Evolution, properties and functional interactions of satellite DNA sequences, Miroslav Plohl
11. Molecular mechanisms of immortalization and cellular aging, Ivica Rubelj
12. Molecular regulation of plant development, Branka Salopek-Sondi
13. Transcriptional regulation in eukaryotes, Mary Sopta
14. Serotonergic transmission: genes, proteins and behavior, Jasminka Štefulj
15. Evolution and function of fast evolving portion of eukaryotic genome, Đurđica Ugarković
16. Fundamental molecular studies of *Streptomyces* biology, Dušica Vujaklija
17. Regulation of the cytoskeleton dynamics in cell motility and cytokinesis, Igor Weber
18. Molecular mechanisms of DNA recombination and repair, Davor Zahradka

Research, developmental and international projects

1. Thymistern, Mariastefania Antica (EC FP7 HEALTH-2013-INNOVATION-1, Proposal No: 602587-2, project coordinator: C. Blackburn, UK)
2. EpiGeneSys, WP4: Signalling to the Epigenome, Đurđica Ugarković (EC FP7 Network of Excellence)
3. Dissecting complex regulators of photosynthetic energy conversion, Hrvoje Fulgosi (International Center for Genetic Engineering and Biotechnology, CRP/CRO11-01)
4. Protein ADP-ribosylation in a model prokaryote *Streptomyces coelicolor* and human, Andreja Mikoč (Unity through Knowledge Fund 1B, Grant Agreement 2/13)
5. Epigenetics: Bench to Bedside, Đurđica Ugarković (COST Action TD0905)
6. Compound with platinum: Cell response and mechanisms involved in resistance, Maja Osmak (MZOS, bilateral project with Germany, 910-8/11-01/00292)
7. Epigenetics of serotonin signalling: DNA methylation analyses of serotonin transport-

er, monoamine oxidase B and serotonin receptor 2A, Jasminka Štefulj (MZOS, bilateral project with Germany)

8. Platinum complexes with diazenecarboxamides as potential anti-cancer drugs, Anamaria Brozović (MZOS, bilateral project with Slovenia, 910-08/11-01/00212)
9. Fitochemical evaluation and antioxidant capacities of commercial and autohtonous fruit and vegetable varieties, Branka Salopek Sondi (Podravka d.o.o.)
10. Development of DNA markers for identifying commercially important mollusc species *Ruditapes decussatus* in the Adriatic Sea, Branka Mravinac (Adris Foundation)

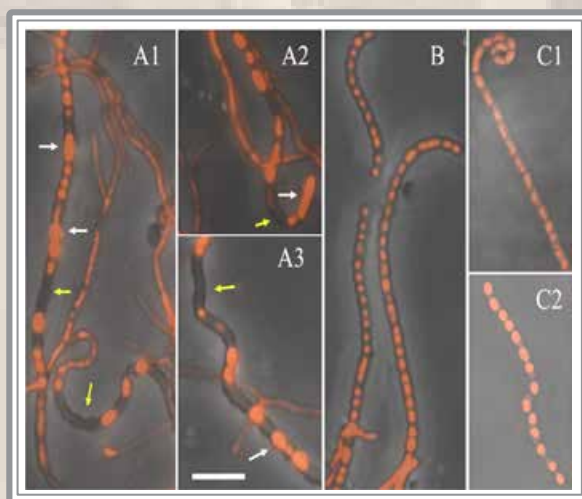


Fig. 4. Segregation defect of the aerial mycelium in the *S. coelicolor* lacking *ssbB*. The aberrant DNA distribution is shown in the spore chains of a mutant (A1-A3), whereas proper segregation can be seen in the wild-type strain M145 (B). White arrows point to the spores with an excessive amount of DNA, and yellow to the compartment lacking DNA. Bar, 5 μ m.

SELECTED INVITED LECTURES

1. Meštrović N: Conserved DNA motifs, including the CENP-B box-like, are involved in satellite DNA array rearrangements. The 19th International Chromosome Conference. Bologna, Italy, September 3-7, 2013.
2. Vujaklija D: Implication of Single Stranded DNA Binding Protein in Chromosome Segregation during Reproductive Growth of *Streptomyces coelicolor*. 4th Central European Fo-

- rum for Microbiology – CEFORM. Keszthely, Hungary, October 16-18, 2013.
3. Plohl M: Genomic composition and turnover of satellite DNA repeats. The 19th International Chromosome Conference. Bologna, Italy, September 3-7, 2013.
 4. Weber I: A dual role model for Rac1 and DGAP1 in cell migration. EMBO Workshop on the Physical Biology of Cancer. Torino, Italy, March 7-10, 2013.
 5. Vujaklija D: How SSB protein ensures sporulation in dominant soil bacteria? Power of microbes in industry and environment. Primošten, Croatia, October 9-12, 2013.
 6. Vujaklija D: Molecular study of dominant soil bacteria: streptomycetes in nature and application to biotechnology. The 2nd International Symposium "Vera Johanides" – Biotechnology in Croatia by 2020. Zagreb, Croatia, May 10-11, 2013.

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1. Paradzik T, Ivic N, Filic Z, Manjasetty BA, Herron P, Luic M, Vujaklija D. Structure-function relationships of two paralogous single-stranded DNA binding proteins from *Streptomyces coelicolor*: implication of SSB-B in chromosome segregation during sporulation. *Nucleic Acids Res* **41** (2013) 3659.
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7. McFall-Ngai M, Hadfield MG, Bosch TC, Carey HV, Domazet-Lošo T, Douglas AE, Dubilier N, Eberl G, Fukami T, Gilbert SF, Hentschel U, King N, Kjelleberg S, Knoll AH, Kremer N, Mazmanian SK, Metcalf JL, Nealson K, Pierce NE, Rawls JF, Reid A, Ruby EG, Rumpho M, Sanders JG, Tautz D, Wernegreen JJ. Animals in a bacterial world, a new imperative for the life sciences. *Proc Natl Acad Sci U S A* **110** (2013) 3229.
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9. Šestak MS, Božičević V, Bakarić R, Dunjko V, Domazet-Lošo T. Phylostratigraphic profiles reveal a deep evolutionary history of the vertebrate head sensory systems. *Front Zool* **10** (2013) 18.

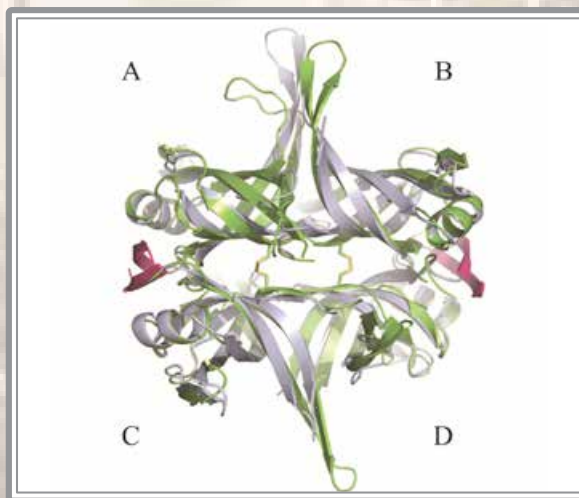


Fig. 5. The first example of crystal structures of two paralogous SSB proteins, SsbB-green and SsbA-grey, from the same organism. The 3D structure of SsbB shows a unique interconnection by two S-S bridges (yellow sticks) between the A/B and C/D subunit pairs.

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1. Zahradka K, Zahradka D (2013). Reckless DNA degradation. In: Brenner's Encyclopedia of Genetics, Maloy S, Hughes K (eds.), San Diego, Academic Press, pp 72-74.
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Division of Molecular Medicine

<http://www.irb.hr/en/str/zmm>

DIVISIONAL ORGANIZATION

Head: Oliver Vugrek

The Division of Molecular Medicine (ZMM) consists of the following laboratories:

- ⇒ Group for Translation Medicine, Oliver Vugrek
- ⇒ Laboratory for Epigenomics, Koraljka Gall Trošelj
- ⇒ Laboratory of Experimental Hematology, Immunology and Oncology, Jelka Gabrilovac
- ⇒ Laboratory of Experimental Therapy, Marijeta Kralj
- ⇒ Laboratory for Hereditary Cancer, Sonja Levanat
- ⇒ Laboratory of Molecular Endocrinology and Transplantation, Mirko Hadžija
- ⇒ Laboratory of Molecular Neuropharmacology, Silva Katušić Hećimović
- ⇒ Laboratory of Molecular Neuropsychiatry, Dorotea Mück-Šeler
- ⇒ Laboratory of Molecular Virology and Bacteriology, Magdalena Grce
- ⇒ Laboratory of Molecular Oncology, Jasminka Pavelić
- ⇒ Laboratory for Oxidative Stress, Neven Žarković
- ⇒ Laboratory for Personalized Medicine, Sanja Kapitanović
- ⇒ Laboratory for Reactive Radicals, Tihomir Balog
- ⇒ Laboratory for Systems Biomedicine, Mario Cindrić
- ⇒ Animal Facility Unit, Ranko Stojković



OVERVIEW OF THE DIVISION

The mission of the DMM is further affirmation as a center of expertise and innovation to become a dynamic actor in the European Research Area (ERA), and to foster leadership in regional economic and social sustainable development to overcome challenges to advanced health care for the benefit of actual and future patients.

These strategic objectives are tackled through the Division's presence in international competitive projects (FP7, IPA, UKF, and bilateral projects). A major breakthrough to achieve these goals was success in obtaining funds from three major sources, e.g. the Instrument for Pre-Accession Assistance (IPA), the Unity Through Knowledge Fund (UKF), and the Seventh Framework Programme of the European Union in 2013. The accumulated budget of these projects is 5.6 million Euros, and a major part is reserved for setting up the most innovative research infrastructure within the RBI. One of the projects, InnoMol is the largest infrastructure FP7 project with the highest budget in natural sciences ever to be conducted in Croatia and the entire amount (4.8 million Euro) is at

the disposal of the RBI and DMM (Vugrek O, project coordinator) to set up the most innovative research infrastructure of personnel and equipment. The goal of the project financed by IPA, RapidCell's (Cindric M, PI) is development of a method of rapid detection of pathogens and tumor cells for use in clinical practice. The project supported by UKF (Katušić Hećimović S, PI) is a competitive research project (200.000 Euro) which aims to elucidate the role of lysosomal dysfunction as a common mechanism of neurodegenerative diseases such as Alzheimer's and Parkinson's disease. Čaušević M and Katušić Hećimović S (project coordinator) have been granted the FP7-PEOPLE-2013-IEF Project BrainProtect to examine presenilin 2 (PS2) protein-mediated molecular and cellular events that are protective against Alzheimer's disease. The goal of the FP7 PRIME-XS-consortium grant project (Vugrek O) is to identify differences in protein-protein interactions and protein signatures between AHCY deficient cell extracts and controls by SILAC-based mass spectrometry analysis. Worthwhile to mention is that all mentioned projects enhance human resources through employment of new experts, and significantly increase mobility of all types of researchers working in the Division.

The DMM intends to extensively apply an interdisciplinary approach to its research using basic methods of genetics, molecular and cell biology, biochemistry, bioinformatics, and biostatistics as well as the use of animal models. The DMM has at its disposal several disease-based models ranging from cancer, neurodegenerative and neuropsychiatric disorders, imprinting and methylation disorders, and others. Deploying the latest 'omics'-approaches such as functional genomics, proteomics, epigenomics, and chemogenomics will allow deciphering major cellular regulatory mechanisms, in particular signal transduction pathways, cell death regulation, protein-protein interaction networks, and post-translational modifications. Accordingly, this will serve as the basis for a global

understanding of molecular processes in both health and disease and how they may be used to facilitate disease prevention, diagnosis and therapy.

The DMM, with its numerous valuable samples collected through long-standing collaborations with clinicians (e.g. in oncology, neurology, psychiatry and others), represents an important biomedical core, which together with the expertise of senior researchers, a large number of Early Stage Researchers (ESR), State-of-the-Art infrastructure, provides all of the required building blocks to excel beyond State-of-the-Art with the potential to steer medical research at a national and international level into new avenues of innovation and technology.

TOP ACHIEVEMENTS

Genotype-independent decrease in plasma dopamine beta-hydroxylase activity in Alzheimer's disease

A decrease in plasma dopamine beta hydroxylase (DBH) activity was detected in early phase Alzheimer's disease (AD), compared to values in the middle and late stages of the disease, as well as to control values (Fig. 1), while the DBH C-970T polymorphism was not associated with AD. The alterations in DBH activity represent a compensatory mechanism for the

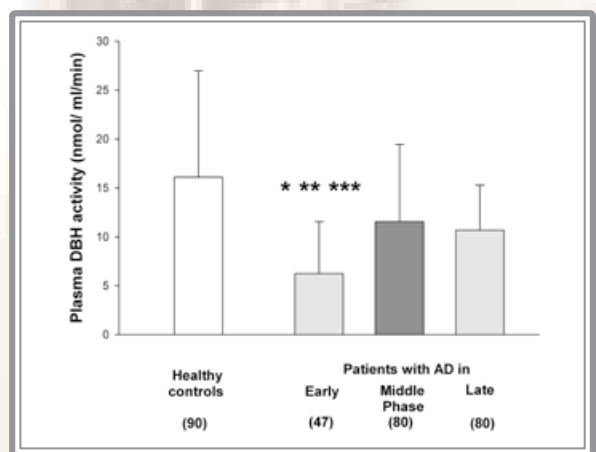


Fig. 1. Plasma DBH activity in patients with different stages of AD and in healthy controls

loss of noradrenergic neurons, and treatment with selective noradrenergic reuptake inhibitors may be indicated in early stages of AD to compensate for the loss of noradrenergic activity (Mustapić et al., 2013).

The association between the catechol-O-methyltransferase (COMT) Val108/158Met polymorphism and hyperactive-impulsive and inattentive symptoms

The functional COMT Val108/158Met polymorphism was significantly associated with hyperactive-impulsive and inattentive symptoms (Fig. 2), which are major subdomains of attention deficit hyperactivity disorder (ADHD). The Met carriers were more frequently found in adolescents with symptoms of hyperactivity or inattention than in subjects without these symptoms. The presence of one or two Met alleles contributed to a risk of developing symptoms of hyperactivity-impulsivity or inattention that may lead to development of ADHD (Nikolac Perković et al., 2013a).

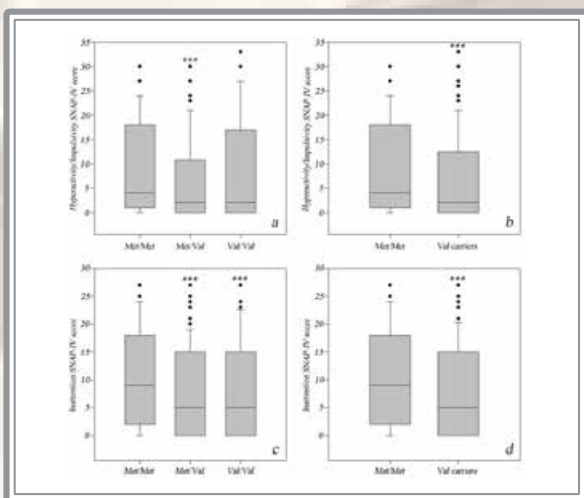


Fig. 2. Association of hyperactivity/impulsivity and inattention symptoms with COMT Val108/158Met polymorphism.

A lack of association between brain derived neurotrophic factor BDNF Val66Met genotypes and

alcohol dependence and/or alcohol-related phenotypes

The Met allele of the brain derived neurotrophic factor (BDNF Val66Met) is a risk allele for depression, suicidal or aggressive behavior. In ethnically homogenous Caucasians no significant differences were found in the frequency of the BDNF Val66Met genotypes or alleles between healthy subjects and alcoholic patients, or when alcoholic patients were subdivided into alcoholic patients with or without various alcohol related phenotypes. Therefore, BDNF Val66Met is not associated with alcohol related depression, aggression, suicidal behavior, delirium tremens, withdrawal syndrome, early/late onset of alcohol abuse and mild or severe alcohol dependence (Nedić et al., 2013).

New insights of interplay between p53 isoforms and p73

We have shown that p53 isoforms can form heterocomplexes with TAp73 and act as dominant-negative inhibitors, but with different efficiency and in a promoter-dependent manner. However, the apoptotic activity of TAp73β was augmented by co-expression of p53β, while other isoforms inhibit its apoptotic activity. The isoforms vary in their half-life and only three isoforms (Δ133p53α, Δ133p53β and Δ40p53) stabilize TAp73β. We contributed in defining the interactions between p53/p73 providing new insight into how the p53 isoforms modulate p73 functions in tumorigenesis (Zorić et al., 2013).

Altering the N-glycan profile of cancer cells in culture

The development of a method for analyzing the N-glycan fraction located at the cell membrane was described. The method is based on incorporation of living cells into polyacrylamide gels, partial denaturation of membrane proteins and subsequent release of N-

glycans with appropriate enzymes followed by HPLC analysis. Using this newly developed method, we revealed multiple effects of several epigenetic inhibitors on the composition of *N*-glycans in human cells. The induced changes were found to be reversible. Since many epigenetic inhibitors are explored as cancer therapeutic agents, where surface glycans play an important role, the work contributes to the understanding of their efficiency in altering the *N*-glycan profile of cancer cells in culture (Horvat et al., 2013).

Deregulated DNA methylation genes in cervical cancerogenesis

Genome wide-analysis of DNA methylation in normal, precancerous and cervical cancer tissue indicated new diagnostic and prognostic gene candidates in cervical carcinogenesis (Fig. 3). Membrane receptors,

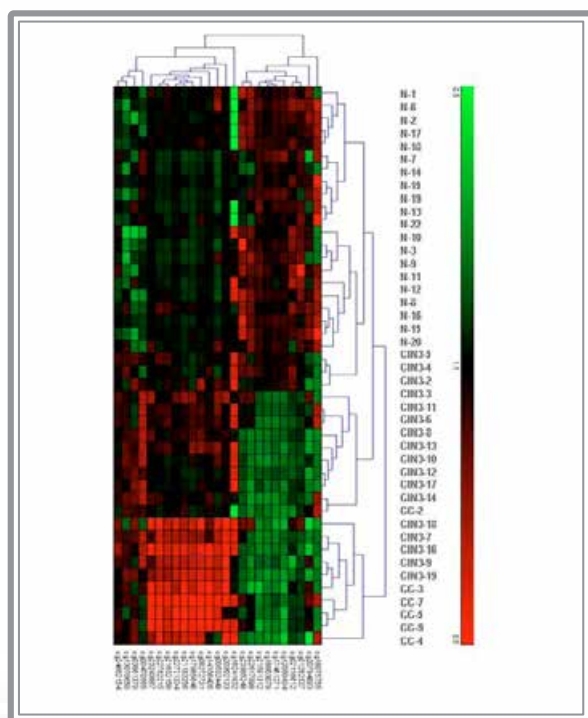


Fig. 3. Unsupervised clustering analysis of the genome-wide DNA-methylation (Infinium Human Methylation 450 BeadChip) in the normal cervical tissue (N), the high grade cervical intraepithelial neoplasia tissue (CIN3), and the cervical cancer tissue (CC). The color gradient green to red displays the β -value ranging from 0-1.

intracellular signaling and gene transcription were epigenetically deregulated by hypermethylation, while the immune system in cancer tissues was extensively affected by hypomethylation (Farkas et al., 2013).

Frequency of HPV detection at different regions of the oral mucosa

Frequency of HPV detection at different regions of the oral mucosa is shown in Fig. 4. The topography of the oral mucosa is coded according to the modified WHO oral topography codes by Roed-Petersen and Roenstrup (Mravak-Stipetić et al., 2013).

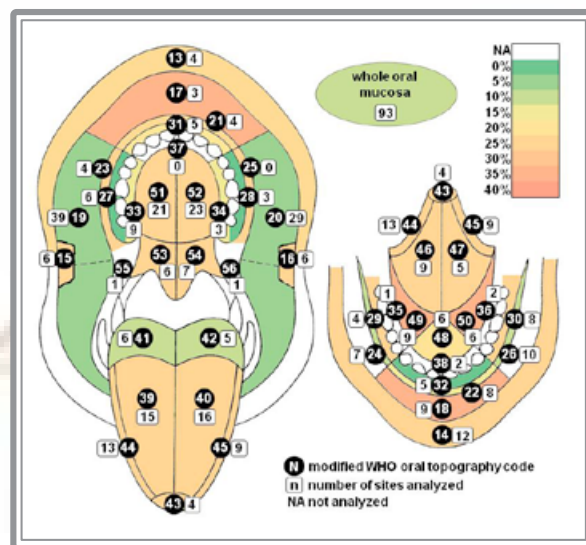


Fig. 4. Frequency of HPV detection at different regions of the oral mucosa

PATENTS

US Patent No. US 8,389,505 B2: Kralj M, Majerski K, Marjanović M, Šumanovac Ramljak T. Adamantane derivatives of aza-crown ethers and their use in treatment of tumor.

NEW EQUIPMENT

1. Confocal microscope Leica SP8 X FLIM
2. Synapt G2-Si HDMS Mass spectrometer and PAL HTS-xt high throughput LC spotting

3. nanoACQUITY UPLC with 2D Technology
4. Thermo Scientific Sorvall Lynx4000 multi-purpose superspeed laboratory centrifuge
5. Diagenode Bioruptor Plus UCD 300-TO Sonication system
6. Beckman Coulter Z2 Series Cell Counter
7. Trans-Blot Turbo Transfer System
8. TECAN HS4800 Hybridization System Station
9. Mixer Mill MM400
10. Sample concentrator SBH200D/3 and gas delivery system SBHCONC/1
11. Differential scanning calorimeter (DSC)
12. Isothermal titration calorimeter (ITC)
13. Microviscosimeter
14. Hyperoxia chamber system for in vitro studies for cell cultures..

AWARDS

Gordana Nedić Erjavec received the Croatian State Reward for young scientists, the most prestigious scientific recognition in Croatia, for significant achievements in the field of biomedicine in 2012.

Nela Pivac received an Award from the Croatian Academy of Sciences and Arts for excellent scientific achievements in the Republic of Croatia for the year 2012 in the field of medical sciences.

Maja Mustapić received financial support for an additional 6-month extension for research training at the University of California, San Diego, Institute for Genomic Medicine.

PROJECTS

Programs supported by the Ministry of Sciences, Education and Sports

1. Integrative genomics and proteomics in cancer research. Krešimir Pavelić
2. Pharmacogenomics, proteomics and psychophysiology of neuropsychiatric disorders. Dorotea Muck-Šeler

Projects supported by the Ministry of Sciences, Education and Sports

1. Cytochrome P450 monooxygenase and tumor appearance in ageing and oxidative stress, Tihomir Balog
2. Gene therapy of tumors by modulating the molecules of the immune system, Jasminka Pavelić
3. The role of nm23 genes in oral squamous cell carcinoma, Maja Herak Bosnar
4. The role of p53/p73 network in soft tissue sarcoma, Neda Slade
5. The mechanism of cholesterol action in the pathogenesis of Alzheimer's disease, Silva Katušić Hećimović
6. Stress, GABA-A receptors and mechanisms of action of neurophychoactive drugs, Du-bravka Švob Štrac
7. The role of different cell death responses to DNA-damage treatment, Marijeta Kralj
8. S-Adenosylhomocysteine hydrolase (AHCY) deficiency: Molecular mechanisms of a new human disease, Oliver Vugrek
9. Role of membrane peptidases on tumor and normal cells, Jelka Gabrilovac
10. Signal transduction in tumors: Hh-Gli interactions and therapeutic potential, Sonja Levant
11. Pharmacogenomics and proteomics of serotonergic and catecholaminergic system, Dorotea Mück-Šeler
12. Molecular basis and treatment of psychiatric and stress related disorders, Nela Pivac
13. Lipids, free radicals and their second messengers in integrative oncology, Neven Žarković
14. Molecular genetics and pharmacogenetics of gastrointestinal tumors, Sanja Kapitanović
15. Proteomic prostate tumor biomarker analysis, Mario Cindrić
16. Obtaining the structures like Langherhans islets from mouse stem cells, Mirko Hadžija
17. Aberrant DNA methylation in HPV associated lesions, Magdalena Grce
18. Epigenetic and immunomodulatory changes in malignant head and neck tumours, Koraljka Gall Trošelj

Research development and international projects

1. Enhancement of the Innovation Potential in SEE through new Molecular Solutions in Research and Development (InnoMol), FP7-REGPOT-2012-2013-1, Oliver Vugrek
2. Rapid Identification of Cells in a Clinical Environment (RapidCell), Mario Cindrić, IPA - Instrument of Pre-Accession assistance: IPA2007/HR/16IPO/001-0404503
3. Lysosomal dysfunction as a common mechanism of neurodegenerative diseases, Silva Katušić Hećimović, Unity through Knowledge Fund
4. BrainProtect— Presenilin 2 - a protector against Alzheimer's disease, FP7-PEOPLE-2013-IEF, Project number 621975, Silva Katušić Hećimović
5. Nonlinear sparse component analysis with applications in chemometrics and pathology, Korpiva I (PI), Croatian Science Foundation, collaborators Marijana Popović Hadžija, Lidija Brkljačić, Marko Filipović; consultants: Mirko Hadžija
6. SILAC analysis of human S-Adenosylhomocysteine hydrolase deficiency, FP7 PRIME-XS-consortium grant, Oliver Vugrek
7. Structure-based drug design for diagnosis and treatment of neurological diseases: dissecting and modulating complex function in the monoaminergic systems of the brain, COST Project, Action CM1103, Dorotea Muck-Šeler, Nela Pivac
8. Detection and tracking of biological markers for early therapeutic intervention in sporadic Alzheimer's disease, Croatian Science Foundation: collaborators: Nela Pivac, Dorotea Muck-Šeler, Maja Mustapić, Matea Nikolac, Gordana Nedić, Dubravka Švob Štrac, Maja Jazvinščak Jembrek
9. Pivac N (2013) Association between gene polymorphisms and pathophysiology of Alzheimer's disease. 7th Croatian Congress of Pharmacology with International Participation, Zagreb, Croatia, September 18-21, 2013.
10. Pivac N (2013) Pharmacogenetics of cardiometabolic side effects of antipsychotics. 14th Central European Neuropsychopharmacological Symposium, Dubrovnik, Croatia, September 25-27, 2013.
11. Muck Šeler D (2013) Serotonergic system and side effects of antipsychotic medication. 14th Central European Neuropsychopharmacological Symposium, Dubrovnik, Croatia, September 25-27, 2013.
12. Muck Šeler D (2013) Alzheimer's disease. COST CM1103 Training School, Istanbul, Turkey, September 9-13, 2013.
13. Muck Šeler D (2013) Treatment of Alzheimer's disease. COST CM1103 Training School, Istanbul, Turkey, September 9-13, 2013.
14. Muck Šeler D (2013) MAO (monoamine oxidase). COST CM1103 Training School, Istanbul, Turkey, September 9-13, 2013.
15. Muck Šeler D (2013) Serotonergic receptors: The new targets in the treatment of Alzheimer's disease. COST CM1103 Interdisciplinary Chemical Approaches for Neuropathology, Valetta, Malta, October 22-25, 2013.
16. Herak Bosnar M, Perina D, Harcet M, Mikoč A, Deželjin M, Četković H (2013) Nme family members in non-bilaterian Metazoans. 9th International Conference of the NDP Kinase/Nm23/awd Gene Family. A new frontier in cell and cancer biology. Boston, Massachusetts, USA, July 31-August 4, 2013
17. Vlanić J, Tlak Gajger I (2013) Antimicrobial activity of honey samples. 3rd National conference on security and quality of bee products - New Trends, Opatija, Croatia, March 22, 2013.
18. Grce M, Dusek D. Evaluation and management of infectious complications in cGVHD, 1st Symposium Chronic Graft Versus Host Disease and long term complications after hematopoietic stem cell transplantation, Zagreb, Croatia, November 15, 2013.
19. Vugrek O (2013) How IPA funds contributed to create infrastructure for development of new tools for basic and applied research. Training workshop on partnership strategies

SELECTED INVITED LECTURES

1. Pivac N (2013) Association between gene polymorphisms and pathophysiology of Alzheimer's disease. 7th Croatian Congress of Pharmacology with International Participation, Zagreb, Croatia, September 18-21, 2013.
2. Pivac N (2013) Pharmacogenetics of cardiometabolic side effects of antipsychotics. 14th Central European Neuropsychopharmacological Symposium, Dubrovnik, Croatia, September 25-27, 2013.
3. Muck Šeler D (2013) Serotonergic system and side effects of antipsychotic medication. 14th Central European Neuropsychopharmacological Symposium, Dubrovnik, Croatia, September 25-27, 2013.
4. Muck Šeler D (2013) Alzheimer's disease. COST CM1103 Training School, Istanbul, Turkey, September 9-13, 2013.
5. Muck Šeler D (2013) Treatment of Alzheimer's disease. COST CM1103 Training School, Istanbul, Turkey, September 9-13, 2013.
6. Muck Šeler D (2013) MAO (monoamine oxidase). COST CM1103 Training School, Istanbul, Turkey, September 9-13, 2013.
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11. Vugrek O (2013) How IPA funds contributed to create infrastructure for development of new tools for basic and applied research. Training workshop on partnership strategies

in developing diagnostic tools "Becoming entrepreneurial: Knowledge transfer from the University of Rijeka Faculty of Medicine to the biotechnology business sector", Faculty of Medicine, Rijeka, Croatia December 6, 2013.

SELECTED ORGANIZED CONFERENCES

1. 7th Croatian Congress of Pharmacology with International Participation, Zagreb, Croatia, September 18-21, 2013 (Pivac N, Muck Šeler D and Švob Štrac D)
2. MSBM 2013 - Mass Spectrometry in Biotechnology & Medicine Summer School, Dubrovnik, Croatia, July 07-13, 2013 (Peter-Katalinić J, Bindila L, Cindrić M, Corthals G, Goodlett DR, Paša-Tolić LJ and Tsybin Y).

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2. Zorić A, Horvat A, Slade N. Differential Effects of Diverse p53 Isoforms on TAp73 Transcriptional Activity and Apoptosis. *Carcinogenesis* **34** (2013) 522.
3. Levatić J, Ćurak J, Kralj M, Šmuc T, Osmak M, Supek F. Accurate Models for P-gp Drug Recognition Induced from a Cancer Cell Line Cytotoxicity Screen. *J Med Chem* **56** (2013) 5691.
4. Farkas SA, Milutin-Gašperov N, Grce M, Nilsson TK. Genome-wide DNA methylation assay reveals novel candidate biomarker genes in cervical cancer. *Epigenetics* **8** (2013) 1213.
5. Muzio LL, Pastorino L, Levanat S, Musani V, Šitum M, Ponti G, Bianchi Scarra G. Clinical utility gene card for: Gorlin syndrome - update 2013. *Eur J Hum Genet* **21** (2013) doi: 10.1038/ejhg.2012.299.
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7. Sagud M, Mihaljević-Peleš A, Uzun S, Vukšan Cusa B, Kozumplik O, Kudlek-Mikulić S, Mustapić M, Barišić I, Muck Šeler D, Pivac N. The lack of association between components of metabolic syndrome and treatment resistance in depression. *Psychopharmacology* **230** (2013) 15.
8. Horvat T, Deželjin M, Redžić I, Barišić D, Herak Bosnar M, Lauc G, Zoldoš V. Reversibility of membrane N-glycome of HeLa cells upon treatment with epigenetic inhibitors. *PLoS One* **8** (2013), e54672.
9. Mravak-Stipetić M, Sabol I, Kranjčić J, Knežević M, Grce M. Human papillomavirus in the lesions of the oral mucosa according to topography. *PLoS One* **29** (2013) e69736.
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11. Nedić G, Nikolac Perković M, Nenadić Svirgin K, Muck Šeler D, Borovečki F, Pivac N Brain-derived neurotrophic factor Val⁶⁶Met polymorphism and alcohol-related phenotypes. *Progr Neuro-Psychopharmacol Biol Psychiatry* **40** (2013) 193.
12. Nikolac Perković M, Pucić Baković M, Kristić J, Novokmet M, Huffman JE, Vitart V, Hayward C, Rudan I, Wilson JE, Campbell H, Polašek O, Lauc G, Pivac N. The association between galactosylation of immunoglobulin G and body mass index. *Progr Neuro-Psychopharmacol Biol Psychiatry* **48** (2013b) 20.
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ed With Haloperidol. *J Clin Psychopharmacol* **33** (2013) 593.

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Review Articles

1. Bortolato M, Pivac N, Muck Šeler D, Nikolac Perković M, Pessia M, Giovanni GD. The role of serotonin at the interface between aggression and suicide. *Neuroscience* **236** (2013) 160.
2. Jazvinščak Jembrek M, Babić M, Pivac N, Hof PR, Šimić G. Hyperphosphorylation of tau by GSK-3 β in Alzheimer's disease: the interaction of A β and sphingolipid mediators as a therapeutic target. *Transl Neurosci* **4** (2013) 466.

CHAPTERS IN BOOKS

1. Pivac N (2013) Biological and genetic theories of eating disorders (in Croatian) In: Eating disorders – from understanding to treatment.

Marčinko D et al.; (Marčinko D, ed), Medicinska naklada, Zagreb, pp 116-121.

2. Pivac N (2013) Molecular basis of behavioral and emotional disorders in children and adolescents (in Croatian), Chapter IV. In: Psychopathology in children and adolescent age. Katarina Dodig Ćurković et al. Dodig Ćurković K (ed), University book of the School of Medicine in Osijek, Svijetla grada and Knjizara Nova Publishers, pp 20-34
3. Pivac N, Nedić G, Kozarić-Kovačić D, Nikolac M, Grubišić Ilić M, Mustapić M, Jendricko T, Rakos I, Muck Šeler D (2013) Biomarkers as new tools to improve the diagnosis and treatment of PTSD. NATO Science for peace programme: NATO ASI - Invisible Wounds, New Tools to Enhance PTSD Diagnosis and Treatment, Wiederhold, Brenda K (ed). Amsterdam: IOS Press, pp 21-72.
4. Švob Štrac D, Mustapić M, Sagud M, Uzun S, Kozumplik O, Presečki P, Nikolac M, Mimica N, Nedić G, Mihaljević Peles A, Pavlović M, Marčinko D, Pivac N, Muck Šeler D (2013) Lipid levels in neuropsychiatric disorders. Triglycerides: Chemical Structure, Biosynthesis and Role in Disease, Araujo C, Perez D (ed), NOVA Sci Publ, pp 1-79.
5. Gall Trošelj K (2013) A Healthy Epigenetic Lifestyle a la Croatia. Centerpoint Now- Sustainability. In: de Gonzaga S (ed) New York: World Council of Peoples for the United Nations. pp: 134-136.

DIVISIONAL ORGANIZATION

Head: Tarzan Legović

The Division for Marine and Environmental Research (DMER) consists of the following laboratories:

- ⇒ Laboratory for Aquaculture and Pathology of Aquatic Organisms, Damir Kapetanović
- ⇒ Laboratory for Analytical Chemistry and Biogeochemistry of Organic Compounds, Marijan Ahel
- ⇒ Laboratory for Inorganic Environmental Geochemistry, Goran Kniewald
- ⇒ Laboratory for Bioelectrochemistry and Surface Imaging, Vesna Svetličić
- ⇒ Laboratory for Biological Effects of Metals, Marijana Erk
- ⇒ Laboratory for Physical Chemistry of Traces, Milivoj Lovrić
- ⇒ Laboratory for Physical Chemistry of Aquatic Systems, Irena Ciglencečki Jušić
- ⇒ Laboratory for Informatics and Environmental Modelling, Tarzan Legović
- ⇒ Laboratory for Molecular Ecotoxicology, Tvrtko Smital
- ⇒ Laboratory for Radioecology, Delko Barišić
- ⇒ Laboratory for Satellite Oceanography, Milivoj Kuzmić



OVERVIEW OF THE DIVISION

Our mission in the Division is to expand and deepen our leadership in fundamental and applied studies of environmental systems, processes and states. Our research is oriented toward the optimization of environmental management for the benefit of our country and the world.

During 2013, division scientists worked on more than 50 research projects contracted by the Ministry of Science, Education and Sport and outside clients. These projects spanned a wide range of topics in marine and environmental science, ranging from satellite oceanography down to nanotechnology. Research results were published in 72 scientific papers in journals indexed by Current Contents with an additional 11 papers accepted for publication. The majority of papers were published in journals above the mean impact factor for environmental sciences. In addition, 17 papers were published in other non-indexed scientific journals. Our scientists gave 18 invited lectures, helped organize 4 conferences, were engaged in running 4 Ph.D. and one undergraduate school. In addition 2 Ph.D. theses were defended under the mentorship of division scientists. Finally, 23 undergraduate

and 76 post-graduate courses were given at universities in Croatia and abroad. All of the given courses were among the best given at participating universities.

TOP ACHIEVEMENTS

Molecular characterisation and infection dynamics of *Dentitruncus truttae* from trout (*Salmo trutta* and *Onchorhynchus mykiss*) in the Krka River, Croatia.

An epidemiological study of *D. truttae* from trout (*Salmo trutta* and *Onchorhynchus mykiss*) in the Krka River, showed specific seasonal (higher parasite abundance in autumn) and spatial distributions (higher abundance at the upstream sampling sites) as well as the association of parasite dynamics with fish sex (higher abundance in male than female trout). The haplotype frequency distribution and intrapopulation genetic variation revealed minimal genetic variability within *D. truttae* population from the Krka River, in contrast to certain previously studied acanthocephalans. Phylogenetic analysis confirmed the taxonomic grouping of *D. truttae* in the Illiosentidae family first made more than 50 years ago based on morphology (Vardić Smrzlić et al., 2013).

Title occurrence, characterization and antimicrobial susceptibility of *Vibrio alginolyticus* in the Eastern Adriatic Sea.

V. alginolyticus was the only isolated *Vibrio* species from both marine water and fish samples, without significant differences between these isolates. Thus it is the main pathogen for aquaculture in the Adriatic Sea. The occurrence of *V. alginolyticus* was strongly correlated to ambient temperature (i.e. sampling season), where antimicrobial sensitivity showed high susceptibility to flumequine, chloramphenicol and oxytetracycline, and resistance to ampicillin, penicillin,

piperacillin, sulfamethoxazole/trimethoprim and trimethoprim (Kapetanović et al., 2013).

Importance of considering fish intestinal parasites, the acanthocephalans, in metal exposure assessment

Two acanthocephalan species, *Pomphorhynchus laevis* and *Acanthocephalus anguillae* were examined in 59 specimens of European chub (*Squalius cephalus* L.) sampled at 5 locations along the Sava River in Croatia. The highest accumulation in both acanthocephalan species was found for non-essential metals and followed the order: Ag>Pb>Cd. Notably in the river section with low metal contamination, parasitism affected metal levels, resulting in lower Cu, Cd and Pb concentrations in chub infected with *P. laevis* than in uninfected chub. Higher Cu and Cd levels in *P. laevis* suggests that acanthocephalans can be sensitive bioindicators when low metal levels have to be detected (Filipović Marijić et al., 2013).

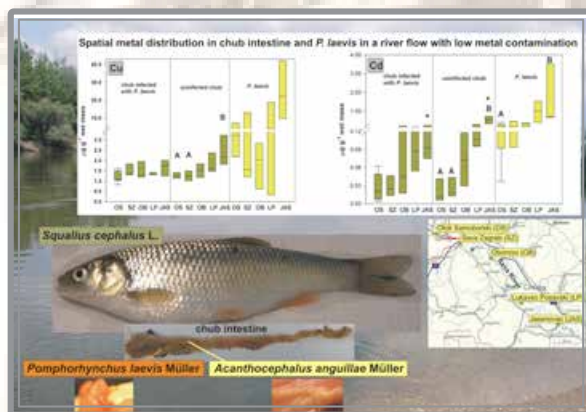


Figure 1. Effect of acanthocephalan infection on metal, total protein and metallothionein concentrations in European chub from a Sava River (Filipović Marijić et al., 2013)

Distribution and chemical speciation of arsenic and heavy metals in highly contaminated waters

Determination of the distribution and chemical speciation of arsenic and heavy

metals in five acidic springs and in the receiving river near Srebrenica (Bosnia and Herzegovina) used for centuries for health-care purposes, was carried out. Although a small discharge, spring waters caused a decrease in the receiving river pH (from 7.3 to 3.4) and a considerable increase in the concentrations of elements. The enrichment factor for the studied elements ranged from 1.2 for Sr up to 425 for As. Complexation of dissolved metals by organic matter was predicted to be significant only for the two river sites with neutral pH (Lenoble et al., 2013).



Figure 2. Multiprobe measurements (left), voltammetric measurements (right) in Bijela Rijeka River, near Srebrenica, Bosnia and Herzegovina (Lenoble et al., 2013)



Figure 3. Sampling at the Bijela Rijeka River near Srebrenica, Bosnia and Herzegovina (Lenoble et al., 2013)

Identification and on line monitoring of reduced sulphur species (RSS) by voltammetry in oxic waters

Based on automatic on-line measurements, identification of Reduced Sulphur Species (RSS) in oxic waters was performed

applying cathodic stripping voltammetry (CSV) with the hanging mercury drop electrode (HMDE). Pseudopolarographic studies accompanied with increasing concentrations of copper revealed the presence of elemental sulphur S(0), thioacetamide (TA) and reduced glutathione (GSH) as the main sulphur compounds in the investigated river (Superville et al., 2013).

Electrochemical detection and sizing of nanoparticles

TA cheap and reliable coulometric method is used for efficient detection and sizing of metallic nanoparticles. In order to determine the basic properties of nanoparticles, the shape, intensity, duration and number of signal spikes formed by impact of nanoparticles with a micro-electrode were analysed with specifically developed software. The method was successfully applied to the analysis of silver and Fe₃O₄ nanoparticles in model solutions, as well as in environmental media (Lees et al., 2013; Stuart et al., 2013; Tschulik et al., 2013).

Application of the complex Effects-Directed Analyses (EDA) of contaminated sediment samples

The study is the first report to identify nonionic surfactants of the alcohol polyethoxylate type and polypropylene glycols as potent inhibitors of fish P-gp activity. These nonionic surfactants were major constituents of contaminated sediment extracts, exhibiting strong fish P-gp inhibitory potency. Consequently, although surfactants are generally considered only weakly to moderately toxic at the concentrations typically found in the aquatic environment, the results from this study reveal their potential to modulate the toxicity of other xenobiotics by inhibiting efflux activity of the fish P-glycoprotein. The presented findings indicate the need for a careful re-assessment of the ecotoxicological relevance of these ubiquitous environmental contaminants (Žaja et al., 2013).

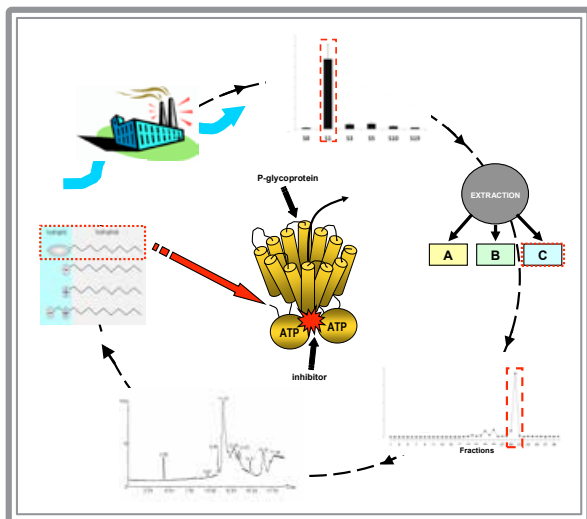


Figure 4. Effects-Directed Analyses (EDA) scheme used in the study (Zaja et al., 2013.)

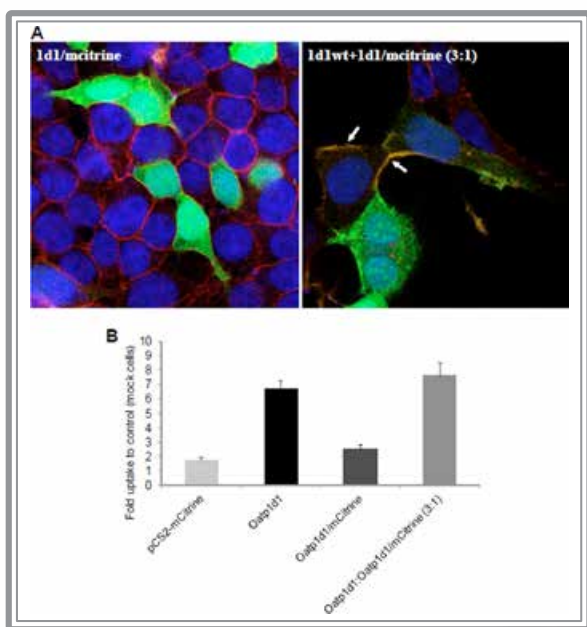


Figure 5. A: cell localization of Oatp1d1 tagged on the N terminus with mCitrine (1d1/mCitrine) and cotransfection of Oatp1d1 without mCitrine and with mCitrine tag; B, uptake of model Oatp1d1 substrate Lucifer Yellow into the Oatp1d1-overexpressing cells. (Popović et al., (2013).

EDUCATION

The following four Ph.D. programmes were coordinated by the Division: **Environmental Management** and **Oceanology** with the University of Zagreb; **Biophysics** with the University of Split; and **Environmental**

Protection and Nature Conservation with the University J.J. Strossmayer in Osijek. In addition, our scientists helped coordinate the **Marine Sciences** undergraduate and graduate school with the University of Pula.

A total of 23 undergraduate and 76 post-graduate courses were given at universities in Croatia and abroad. As revealed by anonymous student evaluations, all of the given courses were among the best at participating universities.

AWARDS AND APPOINTMENTS

1. Željka Fiket, 2013 L'Oreal Prize for Women in Science.
2. Marta Popović, The "Željko Trgovčević" award by the Croatian Genetic Society for the best research article published in 2013 by a young scientist.
3. Tarzan Legović, The Best Paper, Special Awards Certificate. International Scientific Conference on Advanced Information Technologies and Scientific Computing, Samara State Aeronautical Institute, Samara, Russia, December 7, 2013.
4. Tarzan Legović, member, Compliance Committee, Barcelona Convention, Mediterranean Action Plan, Athens, Greece.
5. Tarzan Legović, Vice-president, State Committee on interdisciplinary science, Ministry of Science, Education and Sport, Zagreb.

PROJECTS

Programs supported by the Ministry of Science, Education and Sports

1. Biogeochemical Processes and Environmental Risk, Marijan Ahel

Projects supported by the Ministry of Science, Education and Sport

1. Organic compounds as molecular biomarkers of antropogenic impact, Marijan Ahel
2. Metal-induced cellular changes in aquatic organisms, Marijana Erk

3. Radionuclides and trace elements in environmental systems. Delko Barišić
4. Nature of organic matter, interaction with traces and surfaces in environment, Irena Ciglencić-Jušić
5. Mathematical modeling of circulation and satellite sensing of boundary processes, Mili-voj Kuzmić
6. Pathology of aquatic organisms in relation to pollution and aquaculture, Damir Kapetanović
7. Electroactive films for ecologically acceptable energy conversion and storage, Višnja Horvat-Radošević
8. Electroanalytical research on microcrystals and traces of dissolved substances, Milivoj Lovrić
9. Interactions of trace metal species in an aquatic environment, Ivanka Pižeta
10. Ecotoxicological significance of ABC transport proteins in aquatic organisms, Tvrtko Smital
11. Surface forces on atomic scale applied in marine science and nanotechnology. Vesna Svetličić
12. Biogeochemistry of metals in sedimentary systems and soils in Croatia, Goran Kniewald
13. Ecological modelling for sustainable management of resources, Tarzan Legović
14. Information systems for environmental quality and risk assessment, Jadranka Pečar-Ilić
15. Networked Economy, Jadranka Pečar-Ilić
16. Development of a nanotechnology-based targeted recognition system for bio-macromolecules, Croatian Science Foundation (2010-2014), Project leader: D. Lyons
17. Systematic study of the Adriatic Sea as a basis for sustainable development of the Republic Croatia, Croatian National Monitoring Programme of the Adriatic Sea.

Selected research, developmental and international projects

1. Croatian-Macedonian bilateral project: Bacterial and parasitical communities of chub as indicators of the status of environment exposed to mining activities, Damir Kapetanović
2. Bilateral Croatian-(FYR) Macedonian proj-

ect: "The assessment of metal availability and effects on feral fish in the rivers under the impact of mining activities" (Croatian partner: RBI, DMER, Laboratory for biological effects of metals, project leader: Zrinka Dragun; FYR-Macedonian partner: Faculty of Natural Sciences and Mathematics, Ss. Cyril and Methodius University in Skopje, project leader: Maja Jordanova).

3. Bilateral Croatian-French project (Cogito): "Intracellular mapping of essential and nonessential trace elements in the organs of indigenous fish by NanoSIMS" (Croatian partner: RBI, DMER, Laboratory for biological effects of metals, project leader: Zrinka Dragun; French partner: University of Pau/CNRS, Institute of Analytical Sciences & Physical-chemistry for Environment & Materials (IPREM), project leader: Dirk Schaumlöffel).
4. Biogeochemical characterization of ecotoxic metals in marine lake Mir – PP Telašćica, Marina Mlakar
5. Anchialine cave Čapljina, supported by The Šibenik-Knin County and HAZU, Neven Cukrov
6. Croatia-Slovenia bilateral project, Calibrations of paleoenvironmental records in (sub) recent tufa, Neven Cukrov
7. Study of electrochemical methods for the detection of trace metals in seawater, French defence agency (DGA), Leader: C. Garnier; CRO Collaborators: D. Omanović, I. Pižeta and M. Lovrić.
8. Development of nanotechnology-based sensor for bio-molecules (Croatian Science Foundation). Team leader Vesna Svetličić.
9. Sensitive measurement, detection, and identification of engineered nanoparticles in complex matrices (SMART-NANO, FP7 Collaborative Project), Team member Vesna Svetličić.
10. European network on applications of atomic force microscopy to nanomedicine and life science. COST Action (2010-2014). WG 4: Environmental Nanotoxicology and Nanoparticles, Coordinator Vesna Svetličić. National representatives: Vesna Svetličić and Galja Pletikapić.
11. Electrotransfer of plasmid DNA in vesicles and cells by application of atomic force mi-

- croscopy, electrochemical methods and mathematical modeling, Croatia-France Program "Cogito" Partners Hubert Curien, Nadica Ivošević DeNardis.
12. Impact assesment and determination of organic pollutants in the waters of the Boka Kotorska, Croatia-Montenegro bilateral co-operation in science and technology, Nadica Ivošević DeNardis.
 13. Interaction of ligand coated nanoparticles with the lipid membranes, Croatia- Germany bilateral cooperation (DAAD), Suzana Šegota.
 14. Establishing and developing of an ecotoxicology platform in Serbia and Croatia: a focus on zebrafish (*Danio rerio*), Tvrtko Smital – Swiss National Science Fondation (SNSF), SCOPES 2009-2013: Joint Research Project;
 15. EDA-EMERGE - Innovative biodiagnosis meets chemical structure elucidation – Novel tools in effect directed analysis to support the identification and monitoring of emerging toxicants on a European scale, Marijan Ahel (2011-2013) – Marie Curie Initial Training Networks (ITN) project.
 16. Carrying capacity for visitors to the National Park Krka, NP Krka, Šibenik, Tarzan Legović
 5. Kniewald G. Integrated coastal zone management issues in karstic estuarine environments. International Congress on Geology and Geophysics (ICGG-2013), Beijing, China, June 14-18, 2013.
 6. Kniewald G. The Krka river watershed – geological structure and environmental management issues. 21st International Symposium on Environmental Biogeochemistry, Wuhan, China, October 13-18, 2013.
 7. Legović T. Principles concerning maximum sustainable yield in ecosystems. International Society for Ecological Modelling Conference, Toulouse, France, October 28-31, 2013.
 8. Legović T. Principles of maximum sustainable yield in ecosystems. International Scientific Conference on Advanced Information Technologies and Scientific Computing, Samara State Aeronautical Institute, Samara, Russia, December 4, 2013.
 9. Pletikapić G. Standardization of nanoparticle size measurement using atomic force microscopy. Workshop Standardization: Imaging single molecules and nanoparticles; Force Spectroscopy related to the COST Action TD1002 programme Dijon, France, July 3-5, 2013.
 10. Pletikapić G. Standardization of nanoparticle size measurement using atomic force microscopy. Workgroup meeting on Standardization and Education related to the COST Action TD1002 programme, Dubrovnik, Croatia, September 26-27, 2013.
 11. Šegota S. Biophysical behaviour of lipid membranes in interaction with nanoparticles in physiological and seawater media. Karlsruhe Institute of Technology, Karlsruhe, Germany, November 5, 2013.
 12. Svetličić V. AFM as a tool in marine ecology, MESA+ Institute for Nanotechnology, University of Twente, Netherlands, March 2013.

SELECTED INVITED LECTURES

1. Ciglencčki-Jušić I. Rogoznica Lake (Croatia), A unique anoxic seawater system on the Adriatic coast, University of Ancona, Dept. Life and Environmental Sciences. Ancona, Italy, June 2013.
2. Frka-Milosavljević S. Physico-chemical properties of surfactants in different environmental compartments. GEOMAR-Helmholtz Centre for Ocean Research, Kiel, Germany, June 17, 2013.
3. Ivošević DeNardis N. Adhesion of lipid vesicles at an electrified interface. Institut de Pharmacologie et de Biologie Structurale, Toulouse, France, September 11, 2013.
4. Ivošević DeNardis N. Electrochemical characterization of marine particles, Institute for marine biology, Kotor, Montenegro, April 23, 2013.

SELECTED ORGANIZED CONFERENCES

1. MERMEX international workshop, related to the French MERMEX ([Marine Ecosystems Response In The Mediterranean Experiment](#))

- project; Rudjer Boskovic Institute, 10-12 June 2013. (Ciglenečki Jušić I)
2. International Society for Ecological Modelling Conference 2013, Toulouse, France, October 28-31, 2013 (Legović T)
3. Vth International Meeting on AFM in Life Sciences and Medicine, 7-11 May, 2013, Shanghai, China (Svetličić V)
4. Training school "AFM in biology – Focus on marine biology", Institute of Biophysics, NRC Genoa, April 16-19, 2013, Genoa, Italy (Svetličić V, Mišić Radić T, Pletikapić G)

SELECTED PUBLICATIONS

1. Contreira-Pereira L, Yücel M, Omanović D, Brulport J-P, Le Bris N. Compact autonomous voltammetric sensor for sulfide monitoring in deep sea vent habitats. *Deep-sea research. Part 1. Oceanogr Res Papers*. **80** (2013) 47-57.
2. Cunliff M, Engel A, Frka S, Gašparović B, Guitart C, Murrell JC, Salter M, Stolle C, Upstill-Goddard R, Wurl O. Sea surface microlayers: a unified physicochemical and biological perspective of the air-ocean interface. *Progr Oceanography* **109** (2013) 104-116.
3. Ćurković L, Otmačić Ćurković H, Salopek S, Majić Renjo M, Šegota S. Enhancement of corrosion protection of AISI 304 stainless steel by nanostructured sol-gel TiO₂ films. *Corrosion Sci* **77** (2013) 176.
4. Filipović Marijić V, Vardić Smrzlić I, Raspor B. Effect of acanthocephalan infection on metal, total protein and metallothionein concentrations in European chub from a Sava River section with low metal contamination. *Sci Total Environ* **772** (2013) 463.
5. Janeković I, Powell BS, Matthews D, McManus MA, Sevadjan J. 4D-Var Data Assimilation in a Nested, Coastal Ocean Model: A Hawaiian Case Study. *J Geophys Res* **118** (2013) 1.
6. Kapetanović D, Vardić Smrzlić I, Valić D, Teskeredžić E. Occurrence, characterization and antimicrobial susceptibility of *Vibrio alginolyticus* in the Eastern Adriatic Sea. *Mar Pollut Bull* **75** (2013) 46.
7. Karavoltzos S, Sakellari A, Makarona A, Plavšić M, Ampatzoglou D, Bakeas E, Dassenakis M, Scoullou M. Copper complexation in wet precipitation: Impact of different ligand sources. *Atmos Environ* **80** (2013) 13.
8. Karavoltzos S, Sakellari A, Strmečki S, Plavšić M, Ioannou E, Roussis V, Dassenakis M, Scoullou M. Copper complexing properties of exudates and metabolites of macroalgae from the Aegean Sea. *Chemosphere* **91** (2013) 1590.
9. Komorsky-Lovrić Š, Novak I. Abrasive stripping voltammetry of myricetin and dihydro-myricetin. *Electrochim Acta* **98** (2013) 153.
10. Lechtenfeld JO, Koch PB, Gašparović B, Frka S, Witt M, Kattner G. The influence of salinity on the molecular and optical properties of surface microlayers in a karstic estuary. *Mar Chem* **150** (2013) 25.
11. Lees J, Ellison J, Batchelor-McAuley C, Tschulik K, Damm C, Omanović D, Compton R. Nanoparticle Impacts Show High-Ionic-Strength Citrate Avoids Aggregation of Silver Nanoparticles. *ChemPhysChem* **14** (2013) 3895.
12. Lenoble V, Omanović D, Garnier C, Mounier S, Đonlagić N, Le Poupon C, Pižeta I. Distribution and chemical speciation of arsenic and heavy metals in highly contaminated waters used for health care purposes (Srebrenica, Bosnia and Herzegovina). *Sci Total Environ* **443** (2013) 420.
13. Lovrić M, Jadreško D, Komorsky-Lovrić Š. Theory of square wave voltammetry of electrode reaction followed by the dimerization of product. *Electrochimica Acta* **90** (2013) 226.
14. Oursel B, Garnier C, Durrieu G, Mounier S, Omanović D, Lucas Y. Dynamics and fates of trace metals chronically input in a Mediterranean coastal zone impacted by a large urban area. *Mar Pollut Bull* **69** (2013) 137.
15. Peintner U, Schwarz S, Mešić A, Moreau P-A, Moreno G, Saviuc P. Mycophilic or Mycophobic? Legislation and Guidelines on Wild Mushroom Commerce Reveal Different Consumption Behaviour in European Countries. *PLoS One* **8** (2013) e63926.
16. Popović M, Žaja R, Fent K, Smital T. Molecular characterization of zebrafish Oatp1d1 (SI-

- co1d1), a novel Organic anion transporting polypeptide. *J Biol Chem* **288** (2013) 33894.
17. Rožmarić M, Rogić M, Benedik Lj, Štrok M, Barišić D. Seasonal and spatial variations of ²¹⁰Po and ²¹⁰Pb activity concentrations in *Mytilus galloprovincialis* from Croatian coast of the Adriatic Sea. *Chemosphere* **93** (2013) 2063.
 18. Stuart EE, Tschulik K, Omanović D, Cullen JT, Jurkschat K, Crossley A, Compton RG. Electrochemical detection of commercial silver nanoparticles: identification, sizing and detection in environmental media. *Nanotechnology* **24** (2013) 444002.
 19. Superville P-J, Pižeta I, Omanović D, Billon G. Identification and on line monitoring of reduced sulphur species (RSS) by voltammetry in oxic waters. *Talanta* **112** (2013) 55.
 20. Tschulik K, Haddou B, Omanović D, Rees NV, Compton RG. Coulometric sizing of nanoparticles: Cathodic and anodic impact experiments open two independent routes to electrochemical sizing of Fe₃O₄ nanoparticles. *Nano Res* **6** (2013) 836.
 21. Vardić Smrzlić I, Valić D, Kapetanović D, Dragun Z, Gjurčević E, Četković H, Teskeredžić E. Molecular characterisation and infection dynamics of *Dentitruncus truttae* from trout (*Salmo trutta* and *Oncorhynchus mykiss*) in Krka River, Croatia. *Vet Parasitol* **197** (2013) 604-613.
 22. Viličić D, Kuzmić M, Tomažić I, Ljubešić Z, Bosak S, Precali R, Djakovac T, Marić D, Godrijan J. Northern Adriatic phytoplankton response to short Po River discharge pulses during summer stratified conditions. *Mar Ecol-Evol Persp* **34** (2013) 451.
 23. Žaja R, Terzić S, Senta I, Lončar J, Popović M, Ahel M, Smital T. Identification of P-glycoprotein (P-gp, Abcb1) inhibitors in contaminated freshwater sediments. *Environ Sci Tech* **47** (2013) 4813.

DIVISIONAL ORGANISATION

Head: Renato Batel

The Centre for Marine Research consists of the following laboratories:

- ⇒ Laboratory for marine molecular toxicology, Bojan Hamer
- ⇒ Laboratory for marine ecotoxicology, Nevenka Bihari
- ⇒ Laboratory for biomineralization nanostructure and radioecology, Davorin Medaković
- ⇒ Laboratory for marine microbial ecology, Mirjana Najdek
- ⇒ Laboratory for processes in the marine ecosystem, Robert Precali
- ⇒ Laboratory for ecology and systematics of benthos, Ana Travizi



TOP ACHIEVEMENTS

Adaptation of marine plankton to environmental stress by glycolipid accumulation

A systematic investigation of non-phosphorus containing glycolipids was conducted in the northern Adriatic Sea. The major finding was that during P-limitation enhanced glycolipid instead of phospholipid accumulation takes place, representing an effective phosphate-conserving mechanism. Also, at seawater temperatures >19 °C autotrophic plankton considerably accumulates glycolipids to achieve thermal stability. High sunlight intensities seem to influence increased glycolipid accumulation. And finally, a substantial portion of CO₂ could be removed from the atmosphere in P-limited regions during summer by its capture by plankton and conversion to glycolipids (Gašparović et al., 2013)

OVERVIEW OF THE DIVISION

The mission of the Center for Marine Research (CMR) is to study processes in the marine environment from the subcellular to the regional scale, especially in plankton and benthic communities of the northern Adriatic Sea. In addition to basic research the CMR is also involved in the monitoring of the Adriatic Sea for government and EU stakeholders, and also participates in several international projects regarding protection of the marine environment.

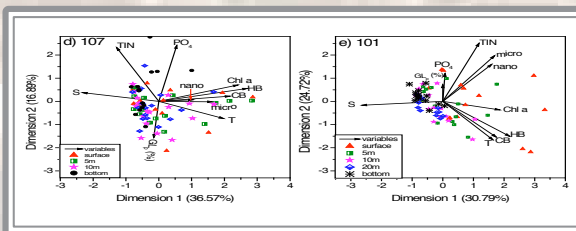


Fig 1. Multivariate analysis of environmental and biological variables in 2008-9 in the northern Adriatic.

Northern Adriatic phytoplankton response to short Po River discharge pulses during summer stratified conditions

Short Po River pulses in August result in surface advection of riverine water, nutrients and phytoplankton from the western to the eastern side of the Adriatic. This surface spreading exhibits inter-annual variability depending on the riverine discharge in the preceding period. The Po River discharge pulse in August 2010 in particular resulted in an extraordinary tongue-like advection of riverine water, nutrients, and phytoplankton towards the eastern Adriatic coast. The phenomenon was detected using both satellite imagery and classical oceanographic measurements (Viličić et al., 2013).

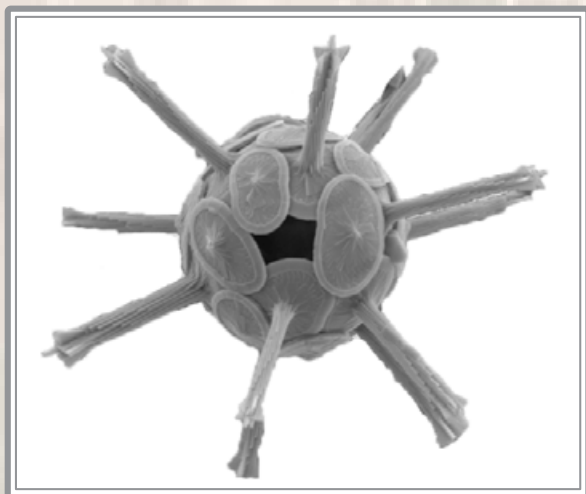


Fig 2. Coccolithophorid *Rhabdosphaera stylifera*, the best indicator of the eastward advection of the Po riverine water in August 2008.

Molecular cross-talk between sponge host and associated microbes

Marine organisms especially those that are sessile, such as sponges, are well known to have specific relationships with a great variety of microorganisms including bacteria and fungi. Sponges produce low-molecular-weight bioactive compounds and secondary

metabolites, to eliminate these microorganisms. In addition, they are armed with cationic antimicrobial peptides allowing them to defend against invasive microorganisms and, in parallel, to kill or repel metazoan invaders as well. The broad range of chemically and functionally different compounds qualifies Porifera as the most important animal phylum to be exploited as a source for the isolation of new potential drugs. The first molecular biological strategies have been outlined to obtain those compounds in a sustainable way, by producing them recombinantly (Wang et al., 2013).

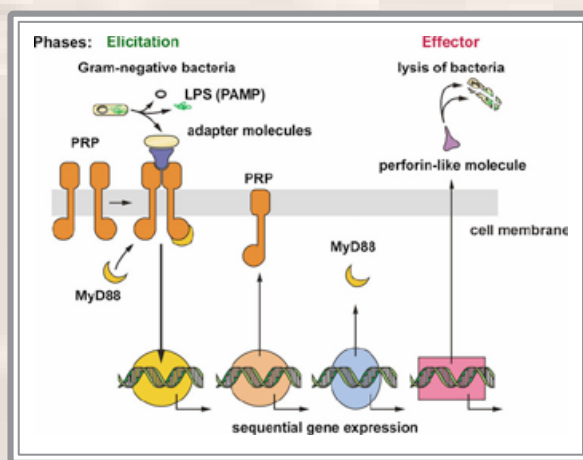


Fig 3. Interaction of sponge cells (*S. domuncula*) with Gram-negative bacteria.

Diets of fan shells (*Pinna nobilis*) of different sizes: fatty acid profiling of digestive gland and adductor muscle

Pinna nobilis is a large bivalve, endemic to the Mediterranean Sea that was shown in a previous study to ingest significantly different proportions of different food items according to its shell height. Based on the analysis of the digestive gland, small *P. nobilis* were associated with a detrital food chain, characterized by saturated and branched-chain fatty acids, while diets of medium and large individuals had a greater proportion of polyunsaturated fatty acids. This likely reflects the fact that smaller individuals feed within the benthic

boundary layer where detritus concentrations are high. Fatty acid incorporation into the adductor muscle, likely representative of food taken up over a longer time period appeared reversed, that is, larger individuals had lower levels of polyunsaturated fatty acids. This most probably reflects energy expenditure, which typically increases with increasing organism size (Najdek et al., 2013).



Fig 4. *Pinna nobilis*.

Structure and variability of a microbial community at a transect crossing a double gyre structure in the north-eastern Adriatic Sea.

The effect of environmental conditions on bacterial community structures, production and enzymatic activities was studied in the north-eastern Adriatic in late spring 2009 in waters belonging to the two gyres, cyclonic (CG) and anticyclonic (AG), and in waters non-affected by the presence of the two gyres. Differences in bacterial community structures and in intensities of cell-specific prokaryotic production and enzymatic activities indicated that CG and AG were isolated cells in which water resided for a different time period. Bulk prokaryotic production and enzymatic activities were significantly lower in the region outside the influence of the gyres. Bacterial communities in these waters, particularly in

deeper layers, were likely introduced by high salinity oligotrophic waters from the central Adriatic (Orlić et al., 2013).

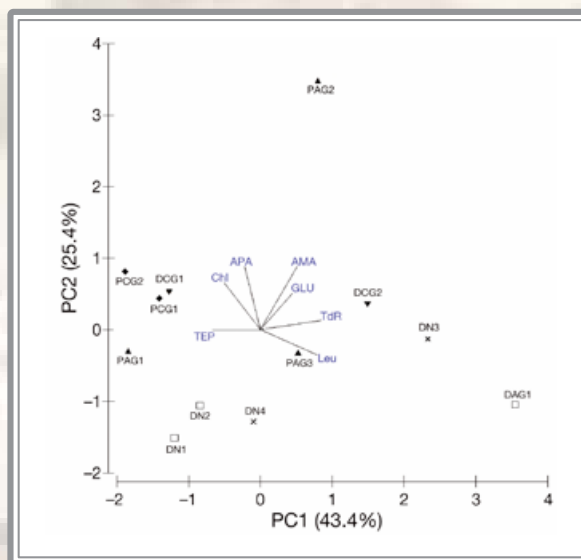


Fig 5. Principal component analysis of late spring 2009 samples.

Sharing biodiversity information globally

The Center for Marine Research (CMR) of the Ruđer Bošković Institute (RBI) became the first Croatian partner and data provider for the DNA Bank Network and the Global Genome Biodiversity Network (GGBN) as well as the Global Biodiversity Information Facility (GBIF), thus making its valuable collection of live cell cultures focused on toxic species, phyto- and zooplankton in

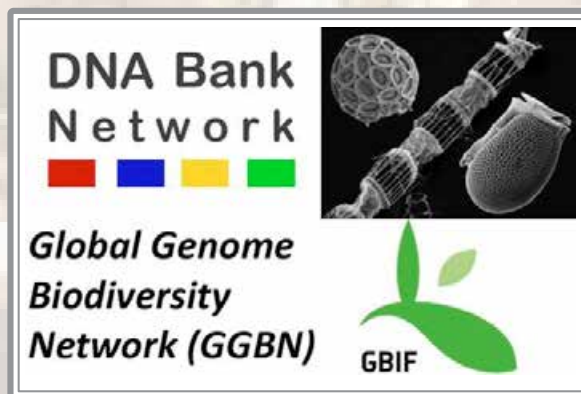


Fig 6. Logos of the organizations and micrograph of phytoplankton species.

the northern Adriatic available to scientists worldwide. Regine Jahn (BGBM) and Martin Pfannkuchen (CMR): Providing Access to the Phytoplankton Biodiversity of the Northern Adriatic Sea: Taxonomy, Systematics, Genetics, Ecology and Open Access Data Management.)

EDUCATION

The Center is involved in the organisation of Marine Sciences Studies (undergraduate) at the Juraj Dobrila University in Pula. The majority of courses are organized by the Center's scientists. Undergraduate and post-graduate courses were also conducted at the Universities of Zagreb, Osijek, Split, and Dubrovnik. Daniela Marić Pfannkuchen defended PhD thesis on 'Potentially toxic diatom genus *Pseudo-nitzschia* in the northern Adriatic Sea: ecological, taxonomic and molecular features' at University of Zagreb, Faculty of Science, Department of Geology.

PROJECTS

Research programs supported by the Ministry of Sciences, education and Sport

1. Impact of pollution on programmed biosynthesis in marine invertebrates, Renato Batel
2. Ecotoxic effect of contamination on marine organisms, Nevenka Bihari
3. Biomineralization processes in marine organisms, Davorin Medaković
4. Structure and physiology of microbial communities in the northern Adriatic front, Mirjana Najdek
5. Mechanisms of long-term changes in the northern Adriatic ecosystem, Robert Precali
6. Biodiversity of benthic communities in the Adriatic: natural and human impacts, Ana Travizi

Research project supported by the Ministry of Sciences, education and Sport

1. SmartNano - Sensitive measurement, detection, and identification of engineered nanoparticles in complex matrices, Daniel Mark Lyons, EC FP7, Contract No. 280779
2. Development of a nanotechnology-based targeted recognition system for bio-macromolecules, Daniel Mark Lyons, Croatian Science Foundation, Project No. 02.05/17
3. FP7-PEOPLE-2011-IAPP Marie Curie Action: Industry-Academia Partnerships and Pathways (coordinators W.E.G. Müller and R. Batel) Marine nanobiotechnology: Manganese oxide-containing core-shell materials formed by proteins from marine organisms for biomedical and environmental applications (CORESHELL). 2011-2015.
4. EU COST Action FA1004: Conservation-physiology of marine fish, (coordinator D. McKenzie, B. Hamer – Croatian representative), 2011-2015.
5. Bilateral cooperation between Croatia and Slovenia (coordinators: B. Hamer/T. Kanduč) Tracing of natural and anthropogenic impacts in marine ecosystem along the Istrian Adriatic coast using the Mediterranean mussel *M. galloprovincialis*. Jožef Štefan Institute, Ljubljana, 2012-2013.
6. Bilateral cooperation between Croatia and Germany (coordinators: M. Pfannkuchen/R. Jahn) Providing access to the phytoplankton biodiversity of the northern Adriatic Sea: Taxonomy, systematics, genetics, ecology and open access data management. Freie Universität Berlin, Botanischer Garten und Botanisches Museum Berlin Dahlem, 2012-2013.
7. FP7-KBBE-2012-6 (coordinators: W.E.G. Müller and R. Batel) BlueGenics – From gene to bioactive product: Exploiting marine genomics for an innovative and sustainable European blue biotechnology industry. 2012-2016.
8. IPA: BALMAS - Ballast water management for Adriatic Sea protection (Croatian coordinator: R. Kraus). 2013-2016.

Organization of conferences, congresses and meetings

1. Coastal Cities Pollution Control Project 2 IBRD 7640/HR –Establishment of a system for monitoring and observation for constant assessment of the Adriatic -1st Scientific-expert workshop. Hotel Eden, Rovinj, 3-7 June 2013.

Invited lectures

1. DM Lyons, Nanomaterials in marine environmental research – from biosensors to nanotoxicology; Croatian Chemical Society, Institute for Agriculture and Tourism, Poreč, Croatia, 12 December 2013.
2. DM Lyons, Nanotechnology and the marine environment: Opportunities and threats; International Summer School of Science, Višnjan Scientific Educational Centre, Croatia, 26 July - 4 August 2013.
3. M. Najdek, Microbial communities associated with marine snow/aggregates. FEMS 2013, 5th Congress of European Microbiologists, Leipzig, Germany, 21-25 July 2013.

SELECTED PUBLICATIONS

1. Gašparović B, Godrijan J, Frka S, Tomažić I, Penezić A, Marić D, Djakovac T, Ivančić I, Paliaga P, Lyons D, Precali R and Tepić N (2013), Adaptation of marine plankton to environmental stress by glycolipid accumulation. *Mar Environ Res* **92** (2013) 120.
2. Viličić D, Kuzmić M, Tomažić I, Ljubešić Z, Bosak S, Precali R, Djakovac T, Marić D and Godrijan J, Northern Adriatic phytoplankton response to short Po River discharge pulses during summer stratified conditions. *Mar Ecol* **34** (2013) 451–466.
3. Wang X, Brandt D, Thakur NL, Wiens M, Batel R, Schroder HC and Muller WEG, Molecular cross-talk between sponge host and associated microbes. *Phytochem Rev* **12** (2013) 369.
4. Najdek M, Blažina M, Ezgeta-Balić D and Peharda M, Diets of fan shells (*Pinna nobilis*) of different sizes: fatty acid profiling of digestive gland and adductor muscle. *Mar Biol* **160** (2013) 921.
5. Orlić S, Najdek M, Supić N, Ivančić I, Fuks D, Blažina M, Šilović T, Paliaga P, Godrijan J. and Marić D, Structure and variability of a microbial community at a transect crossing a double gyre structure in the north-eastern Adriatic Sea. *Aquat Microb Ecol* **69** (2013) 193.



ORGANISATION OF THE CENTRE

Head: Karolj Skala

The Centre for Informatics and Computing Science (CIR) consists of the following units:

- ⇒ Optoelectronics and Visualisation Laboratory, Karolj Skala
- ⇒ Department for R&D of ICST systems, Karolj Skala
- ⇒ Department for Information systems, Nikola Pavković
- ⇒ IT Services Department, Nikola Pavković



The Center also provides technical and technological support and maintains basic information services at RBI on the Linux platform.

TOP ACHIEVEMENTS

Improving Accessibility of Distributed Compute Resources

For domain scientists wrangling with the ever increasing size of data and more demanding computer processing tasks, distributed computer resources present a welcome relief. However, these resources are often challenging to use and require significant technical knowledge and time investment. As part of the AISDC project, the Centre put forward a significant effort to improve the accessibility of those resources by developing a set of webbased solutions that simplify researchers interactions with distributed computing resources. By continuing to develop the CloudMan application (<http://cloudman.irb.hr>), which makes it possible to easily procure and configure a functional data analysis

OVERVIEW OF THE CENTRE

The mission of the Centre is to become a leading ICST (Information Communication Science Technology) centre for the research, development and adoption of new computing, visualisation and information processing paradigms and techniques, their scientific dissemination and their application in other scientific disciplines. The Centre supports multidisciplinary and multi-institutional scientific work, based on the eScience platform and through Virtual Organizations, at the national, EU and global level. The Centre is an active part of the European Research Area and participates in several national and EU projects.

platform on a cloud infrastructure, the procured platform delivers a scalable cluster-in-the-cloud and a data analysis environment preconfigured with a number of applications: Galaxy (additionally configured with dozens of bioinformatics tools and reference genome data), Hadoop, HTCondor.

To promote the reach of CloudMan, the group is developing an ecosystem of tools to further enhance the accessibility of distributed compute resources. The group developed a web application, available at biocloudcentral.org, to simplify the process of starting CloudMan clusters. To support the notion of automation of a predefined data analysis process, we also developed a programming library, called BioBlend (bioblend.readthedocs.org), for programmatically interacting with CloudMan clusters and the Galaxy applications. The developed ecosystem of tools is utilized around the world for research and training purposes by dozens of researchers and groups.

Scientifically, the group is continuing to extend its reach by adopting new technologies. With the Medical University of Innsbruck, we have received a collaborative bilateral grant to explore the capacity of Big Data analysis tools in the context of CloudMan. The members of this group have delivered a number of presentations and training workshops around the world, promoting their results.

CIR has continued its work on the development of the Application specific gateways for distributed computing infrastructures, AdriaScience portal (<http://adria-sci.irb.hr:8080/liferay-portal-6.1.0/>) for advanced ecological predictions through its collaboration on the SCI-BUS EU FP7 project (<http://www.sci-bus.eu>). The portal provides an easy and intuitive web-based user interface for easy and intuitive preparation and execution of meteorological simulations on different national computing infrastructures such as National Grid Infrastructure (CRO-NGI) and HPC cluster Isabella. Currently, the portal supports a Weather Research and Forecasting (WRF-ARW) modelling system for advanced meteorological predictions.

We also completed the development of the AdriaScience portal for advanced meteorological prediction, which is now in the production phase. Another top achievement is the Embedded Electronics Learning Platform (E2LP), an EU FP7 funded project focused on creating a unified learning platform for studies of embedded systems. The Centre for Informatics and Computing is the leader of the project's work package 5. The goal of this WP is to define, build and implement the E2LP start-up kit with a library of illustrative laboratory examples covering the E2LP learning objectives.

CIR coordinated the effort of collecting and implementing laboratory exercises between project partners, and also implemented several new exercises. As a result, the start-up kit currently comprises 67 exercises, divided among three levels by our defined taxonomy: basic exercises, problem solving and projects. Each exercise includes an introduction and motivational part, theoretical background, a practical part of the exercise, a discussion on expected results, as well as other informative components. The complete start-up kit is published and available online.



Fig. 1. Embedded Electronics Learning Platform (E2LP) at RIDE Exhibition on Mipro 2013, Opatija

Furthermore, as part of the CIR's RIDE Exhibition at the international conference Mi-pro 2013, CIR was involved in disseminating E2LP information through poster presentations at a dedicated booth.

COST IC0805 and COST IC1305 projects

The Centre actively participated in the Open European Network for High Performance Computing on Complex Environments COST IC0805 action. Using homogeneous high performance computers different fields of science and engineering solved complex and challenging problems.

We also initialized the project COST IC1305 Network for Sustainable UltraScale Computing (NESUS) which will deal with the development of large (UltraScale) computer systems that are as much as two to three times more powerful than today's systems. Research within the project, involving working partners from 26 European countries over the next four years, should bring multiple benefits to researchers in the field of biology, astrophysics, climate change, energy and ICT.

Dynamic 4D Thermography Imaging System

We continue to develop the novel concept of the standardisation of human body 3D thermal models, captured by multi-resolution real-time 3D thermal imaging system. The standardisation procedure consists of four different processes: Skeleton Detection, Skeleton Transformation, Vertex Deformation and Thermal Texture Mapping process. We presented a concept of 3D thermal model standardisation enabling novel and practical methods for model comparison and analysis.

Basic IT service and maintenance

The helpdesk is continuing its usage of the OTRS Ticketing System which has shown itself to be an indispensable tool for our every-

day operations. All basic services continue to function without any interruptions. The IRB webpage continues to show a steady increase both in unique visitors as well as in the number of visits. The IRB web site is being monitored by our own local open-source AWStats system and Google Analytics.

NEW EQUIPMENT

We installed a DIY MaxCard, Vectis-lite dataflow engine and MaxelerCompiler in the MAX-UP university program and provided access to Data Flow Computing architecture that will be used to address the Big Data problem of assembly; active research in HPC and Cloud computing and development of novel DNA assembly algorithms.

EDUCATION

CIR provides 3 doctoral courses at Faculty of Electrical Engineering and Computing, Faculty of Graphical Arts at the University of Zagreb and University of Josip Juraj Strossmayer in Osijek.

PROJECTS

Research programs supported by the Ministry of Sciences, Education and Sport

1. Distributed Computing and Visualisation, Karolj Skala

Research projects supported by the Ministry of Sciences, Education and Sport

1. Scientific Visualisation Methods, Karolj Skala

Research, developmental and international projects

1. Embedded Computer Engineering Learning

Platform - E2LP, EU FP7, Grant agreement number: 317882, Karolj Skala

2. Application Information Services for Distributed Computing Environments AIS-DC, EU, FP7, Grant agreement number: 277144, Karolj Skala, Enis Afgan
3. SCientific gateway Based User Support, SCI-BUS, EU FP7, Karolj Skala

SELECTED ORGANIZED CONFERENCES

1. 35th International Convention MIPRO, Conference on distributed computing, visualisation and biomedical engineering systems (DC VIS), Opatija, Croatia, May 22-24, 2013 (Karolj Skala)
2. Research Infrastructure Dissemination Event, RIDE 2013, Opatija, Croatia, May 20-24, 2013 (Karolj Skala)

ADDITIONAL INTERNATIONAL WORKSHOPS

1. Biomedical Data Analysis with Galaxy. European Human Genetics Conference (EHGC), Paris, France, June 8-11, 2013.

2. Running Galaxy on the Cloud. Galaxy Community Conference (GCC) 2013, Oslo, Norway, June 30-July 2, 2013.

SELECTED PUBLICATIONS

1. Sloggett C, Goonasekera N, Afgan E. BioBlend: automating pipeline analyses within Galaxy and CloudMan. *Bioinformatics* **29** (2013) 1685.
2. Skala K, Lipić T, Sović I, Grubišić I, Grbeša I. Toward 3D Thermal Models Standardisation for Human Body in Motion. *Quant Infrared Thermogr J* **10** (2013) 207.

Review articles

1. Skala T, Skala K, Afgan E. Impact of 3D Graphic Structure Complexity to the Rendering Time. *J Circuit Syst and Comp* **22** (2013) 12.

ORGANIZATION OF THE CENTRE

Head: Dražen Vikić-Topić

The NMR Centre consists of the following laboratories:

- ⇒ Laboratory for NMR spectroscopy and modelling, Dejan Plavšić
- ⇒ Glass Laboratory, Andrea Moguš-Milanković



OVERVIEW OF THE CENTRE

The Centre performs scientific research in NMR spectroscopy in the field of organic, bioorganic, inorganic and physical chemistry, and provides scientific services for both the Ruđer Bošković Institute and the academic community as a whole in the Republic of Croatia. The Centre provides educational and professional support to researchers from governmental institutions and the pharmaceutical industry, and participates in higher education at the Universities of Zagreb, Rijeka, Split and Osijek. The equipment in the Centre includes Bruker Avance 300 and 600 MHz NMR spectrometers as well as a Varian Gemini 300 MHz NMR spectrometer located at the Faculty of Pharmacy and Biochemistry of the University of Zagreb.

The Laboratory for NMR Spectroscopy and Modelling performs experimental and theoretical research on organic and bioor-

ganic compounds, organometallic molecules, photochemistry and food chemistry as well as mathematical chemistry and modelling, with the aim of determining bioactive compounds, their structures and property/activity relationships. The Glass Laboratory studies the electrical/dielectric properties of various materials such as super ionic glasses, transition metal phosphate glasses, ionic liquids and dental materials. Additionally, important contributions were made in the development and characterization of new nano-materials and microcrystalline materials produced by induced controlled crystallization.

TOP ACHIEVEMENTS

NMR structure determination and development of NMR techniques

The formation of aggregates containing oxalamide gels with a chiral morphology, hexa- and nonamethylene-bridged Bis(l-Leu-oxalamide) was confirmed by ^1H and NOESY spectra taken at various tempera-

tures. NOE experiments are a very useful technique to gain more information on the organization of gel assemblies (Vinković et al., 2013). Two new adamantynaphthalene derivatives, 1-(2-hydroxy-2-adamantyl)-4-methoxynaphthalene and 1-(2-hydroxy-2-adamantyl)-5-methoxynaphthalene were characterized by NMR spectroscopy. For both derivatives dynamic NMR of diastereotopic spins revealed atropisomerism due to hindered rotation around the C–C bond between the adamantyl and the naphthyl moieties, giving rise to intermediate conformational exchange on the NMR timescale at room temperature (Smrečki et al., 2013).

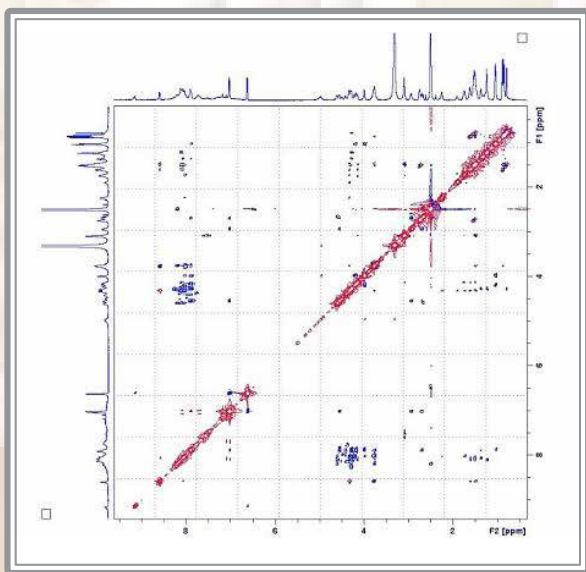


Figure 1. ROESY spectrum of the glycoprotein hormone Erythropoietin.

Molecular modelling

A novel matrix representation of graphs based on the count of equal-distance common vertices to each pair of vertices in a graph was proposed. The element (i, j) of the matrix is defined as the number of vertices at the same distance from vertices (i, j) . The novel matrix is very sensitive to molecular branching and the distribution of vertices in a graph. In particular, ordered row sums of the novel matrix can facilitate solving graph isomorphism for acyclic graphs (Randić et al., 2013).

Food chemistry

We investigated the structure and activity of antioxidant compounds by semi-empirical methods as it relates to their bioactivity. Our results indicated that the active site is responsible for radical inactivation (Lučić et al., 2013).

Influence of germanium oxide addition on the electrical properties of $\text{Li}_2\text{O-B}_2\text{O}_3\text{-P}_2\text{O}_5$ glasses

The increase in dc conductivity with the addition of GeO_2 is attributed to the formation of ion conducting channels arising from the structural modification and formation of P–O–Ge linkages, resulting in an easy migration of Li^+ ions along these bonds. At higher GeO_2 content the glass network became more densely packed and ionic conductivity was slightly hindered as a consequence of the increase of bonding forces inside the network (Moguš-Milanković et al., 2013).

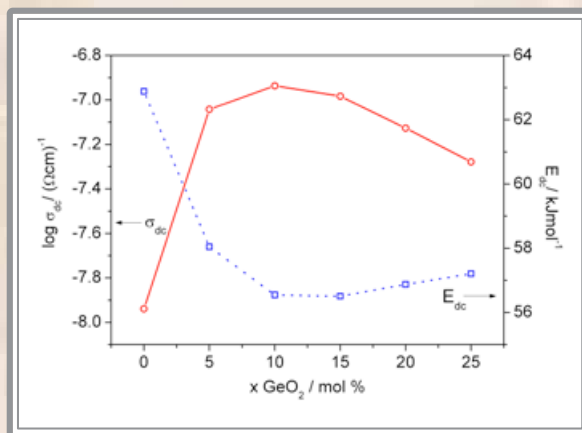


Figure 2. The dependence of the dc conductivity, σ_{dc} , at 303 K and activation energy for dc conductivity upon GeO_2 content.

EDUCATION

Members of the NMR Centre are involved in undergraduate and graduate level courses at the University of Rijeka and University of Zagreb, as well as graduate level courses at

the University of Zagreb, University of Rijeka, University of Osijek and University of Split. Members of the NMR Center also supervised 12 PhD theses at these Universities.

PROJECTS

Projects supported by the Ministry of Science, Education and Sports

1. NMR spectroscopy and modelling of bioactive molecules, Dejan Plavšić
2. Influence of structure on electrical properties of (bioactive) glasses/ceramics, Andrea Moguš-Milanković
3. Modelling of bioactive molecules and testing of their properties and activity, Nikola Štambuk
4. Developing methods for modelling properties of bioactive molecules and proteins, Bono Lučić

Research, developmental and international projects

1. Investigation of relationships between structure and biological activity of polyphenols, bilateral Croatian-Serbian project, Bono Lučić
2. Evaluation of new bioactive materials and procedures in restorative dental medicine (Croatian Science Foundation), Collaborative Research Programmes RBI-IF-School of Dentistry Zagreb, Programme leader: Z. Tarle, RBI project leader: A. Moguš-Milanković
3. Investigation of electrical properties of restorative dental materials (Croatian Academy of Science and Art), 2013/2014 project, Kristina Sklepić
4. Biofactor GmbH, Rudolf Huch Starasse 14, 38667 Bad Harzburg, Germany, developmental project, Nikola Štambuk

5. Nanotemper Technologies GmbH, Flossergasse 4, 81369, Munich, Germany, developmental project, Nikola Štambuk

SELECTED PUBLICATIONS

1. Šijaković Vujičić N, Glasovac Z, Zweep N, van Esch J. H, Vinković M, Popović J, Žinić M. Chiral hexa- and nona-methylene bridged bis(L-Leu-oxalamide) gelators. First oxalamide gels containing aggregates with chiral morphology. *Chem-Eur J* **19** (2013) 8558.
2. Kovač V, Čakić-Semenčić M, Kodrin I, Roca S, Rapić V. Novel ferrocene-dipeptide conjugates derived from aminoferrocene and 1-acetyl-1'-aminoferrocene: Synthesis and conformational studies. *Tetrahedron* **69** (2013) 10497.
3. Randić M, Noviĉ M, Plavšić D. Common. Vertex Matrix: A novel characterization of molecular graphs by counting. *J Comput Chem* **34** (2013) 1409.
4. Moguš-Milanković A, Sklepić K, Blažanović H, Mošner P, Vorokhta M, Koudelka L. Influence of germanium oxide addition on the electrical properties of Li₂O-B₂O₃-P₂O₅ glasses. *J Power Sources* **242** (2013) 91.
5. Androš L, Jurić M, Popović J, Šantić A, Lazić P, Benčina M, Valant M, Brničević N, Planinić P. Ba₄Ta₂O₉ Oxide Prepared from an Oxalate-Based Molecular Precursor – ICharacterization and Properties. *Inorg Chem* **52** (2013) 14299.
6. Štepanić V, Gall Trošelj K, Lučić B, Marković Z, Amiĉ D. Bond dissociation free energy as a general parameter for flavonoid radical scavenging activity. *Food Chem* **141** (2013) 1562.
7. Lučić B, Sović I, Batista J, Skala K, Plavšić D, Vikić-Topić D, Bešlo D, Nikolić S, Trinajstić N. The Sum-Connectivity Index - An Additive Variant of the Randić Connectivity Index. *Curr Comput-Aided Drug Des* **9** (2013) 184.

Head of Library: Bojan Macan

OVERVIEW OF LIBRARY ACTIVITIES

During 2013, the Library continued to promote open access through various activities, disseminating information about open access initiatives among researchers, as well as librarians. The main achievement in this area is the Full-text Institutional Repository of the Ruđer Bošković Institute (FULIR - <http://fulir.irb.hr>), which was successfully launched in 2012. FULIR is the RBI institutional repository in which RBI employees can archive full texts of all types of documents related to their scientific research (full text of articles published in scientific journals, papers published in conference proceedings, graded papers, book chapters, monographs, various reports, presentations and posters presented at conferences), as well as audio-video material and original research data (datasets). The main purpose of FULIR is to gather the whole of RBI's scientific output (published and unpublished) and to present it in open access to the public.

In 2013, further development of the FULIR repository continued. Editing and administration of FULIR were handled by Library staff. Although data input into FULIR is eventually to be based on RBI staff self-archiving, in this initial phase of repository development Library staff handled archiving as well. Since only a small number of RBI scientists have participated in self-archiving thus far, one of the most important tasks for the future is the promotion of FULIR including education and



promotion of both open access and the use of the repository among RBI staff. By the end of 2013, around 900 items were deposited in FULIR. As part of the Library's participation in the OpenAIREplus project, FULIR was made compliant with OpenAIREplus guidelines which made possible the exchange of FULIR records with the OpenAIRE harvester. Preparations were also made on making FULIR compliant with the CROSB (Croatian Scientific Bibliography) database, in order to avoid double input of the same records in databases.



Fig. 1. The Full Text Institutional Repository of the Ruđer Bošković Institute - FULIR

During 2013, the Library continued with its participation in the 7th Framework Programme project called OpenAIREplus (2nd

Generation of Open Access Infrastructure for Research in Europe), together with 41 European partners. The project is intended to facilitate access to the entire Open Access scientific production of the European Research Area, providing links from publications to data. According to plans set out in 2012, the RBI institutional repository FULIR was made compliant with OpenAIREplus guidelines which enables the exchange of FULIR records with the OpenAIRE harvester.

Part of the Library staff continued with individual activities in the FP7 project *Support for Establishment of National/Regional Social Sciences Data Archives (SERSCIDA)*. The project was designed as a strategic project for supporting the cooperation and exchange of knowledge between EU countries associated within the Council of European Social Sciences Data Archives (CESSDA) and Western Balkan Countries in the field of social science data archiving. As part of this project, organizational and technical prerequisites were fulfilled for establishing a Croatian national social science data archive.

The Library continued to provide and monitor input in the Croatian Scientific Bibliography – CROSBIB (<http://bib.irb.hr>). At the end of 2013 CROSBIB included information on some 405.000 papers and other types of work written by Croatian researchers. Preparations were made for making CROSBIB compliant with the RBI institutional repository FULIR. The Library also continued its role in the maintenance of *Who's Who in Science in Croatia* (<http://tkojetko.irb.hr>), which has been used as the basis for collaboration with publisher *Thomson Reuters* and the creation of *ResearcherID* for RBI researchers.

Due to significant cuts in journal subscriptions, the Croatian Centre for Online Databases (<http://www.online-baze.hr>) offered access to fewer databases than in previous years. Access to major publishers' databases such as *Thomson Reuters*, *Elsevier*, *EBSCO* and *Ovid* continued in 2013 in cooperation with the Croatian Ministry of Science, Education and Sports, which subscribed to

these major databases. The Library's collaboration with the University Computing Centre of the University of Zagreb SRCE at the Portal of the Croatian scientific journals HRČAK (<http://hrcak.srce.hr>) continued, resulting in around 350 open access journals included in HRČAK.

Due to a lack of financing, only minor changes in the interfaces, features and database structures of the majority of the above mentioned information services were made. However, planning and preparations for the integration of interoperability tools, monitoring tools and authority tools continued, hopefully to be realized in the next year. Support activities conducted by students of the Department of Information Science at the University of Zadar were invaluable for maintenance of ongoing projects.

COLLECTION DEVELOPEMENT

In 2013 RBI scientists had access to more than 42.000 free and fee journals, around 30 free and fee biomedical and natural sciences databases, as well as 42 biomedical e-books, via subscriptions at the Croatian academic consortia level, and as open access content. Due to ongoing budget cuts to subscriptions at the national level over the past few years, access to many journals was limited to archives, and not to current issues.

In terms of RBI institutional subscriptions, the Library subscribed to 288 journals (subscription to selected titles from different publishers, as well as to journals packages from IOP and Emerald). Quick access to all available journals was provided via the Pero search engine (<http://knjiznica.irb.hr/pero/>) as well as through EZB Elektronische Zeitschriftenbibliothek (<http://lib.irb.hr/web/hr/casopisi/item/202-ezb.html>).

In 2013 the Library acquired 100 new books, a relatively small number due to overall budget cuts. An additional 66 books were donated to the Library from various sources (exchange, international cooperation etc.), of which 11 books were donated by RBI re-

searchers, a valuable contribution to the collection of publications written or edited by RBI researchers. The collection is on display in the Library reading room in the 5th wing.

LIBRARY SERVICES

Bibliometric services

The Library has continued providing bibliometric analysis, primarily for RBI scientists. The Library issued 122 certificates for the purposes of promotion, project applications, scholarships etc. The most requested certificates have been:

- certificates with the number of papers published in journals which are indexed in the Web of Science/Scopus/Current Contents databases;
- citation certificate of papers indexed in the Web of Science/Scopus databases;
- certificate of the Journal Impact Factor for a given year.

In 2013 the Library conducted an extensive analysis of RBI's scientific output for the period of the past 5 years for the purpose of re-accreditation of scientific organisations overseen by the Agency for Science and Higher Education Croatia. Other bibliometric analyses for various purposes were also provided for the whole Institute.

Interlibrary loan

The shortages of the RBI library collections were successfully overcome thanks to the well-established interlibrary loan and lending service with libraries from Croatia and abroad. In 2013 the RBI library received about 1030 requests for document delivery by RBI staff. The majority (814) of these requests were positively resolved, and mostly free of charge thanks to other Croatian libraries and to EURASLIC/IAMSLIC libraries. In addition, the RBI library also received about 382 requests for document delivery from

other Croatian libraries, the majority being positively resolved.

During 2013, phased out the in-house developed Oracle application SEND (Electronic Documents Acquiring System), which was active from 2003-2012. The ILL service was provided via a basic version of SEND. A new SEND application with new functionalities was developed and tested. Its release is planned for the first half of 2014. In addition to RBI Library ILL needs, the new service will also be free to use for other libraries' ILL services.

INTERNATIONAL COOPERATION

The Library continued its international cooperation with EURASLIC (European Association of Aquatic Sciences Libraries and Information Centers) and its parent organization IAMSLIC (European Association of Aquatic Sciences Libraries and Information Centres). Library staff had an active role in EURASLIC activities, as well as in its subgroup ECET (European Countries in Economic Transition). Two members of the library staff participated in the 15th EURASLIC biennial conference in Varna, Bulgaria, May 13-15, 2013. During the Conference, both present members of the Library were appointed to the new board as Executive secretary/website and newsletter editor for the period 2013-2015.



Figure 2: Library staff members during EURASLIC 15th conference in Varna, Bulgaria

The Library also participated in training courses held at the UNSECO/IOC Project Office for IODE in Oostende, Belgium: Ocean-Teacher Academy Training Course on Development and Management of e-Repositories, April 8-12, 2013. Participation was covered by an IODE grant.

ORGANIZATION OF EVENTS

The Library continued to organize the RBI Library Colloquia. Colloquia topics were chosen to be of interest not only to librarians, but also to RBI staff and the general public. In 2013 six colloquia were organized. 108th colloquia was held on October 23rd, during the International Open Access Week, and had a special program during which library staff held several presentations on the OA movement in scientific publishing and OA initiatives in Croatia, including the new portal about OA in Croatia. Several colloquia were organized with online streaming, so there was a “virtual” audience present as well.

The Library has also actively participated in the RBI Open Days event, which was held on April 18-20. Library staff presented library projects, activities and interesting educational online resources at the presentation point called “Pirates in the Library”. The main topic of the presentations were copyright, Open Access, online piracy, Creative Commons etc. As well, the Library was actively involved in organisation of the whole manifestation, having one member in the organization board.

During 2013 the Library also organized a book exchange under the title “Take it or leave it”. RBI employees could bring their used books and exchange them for other books. Besides books, people were also encouraged to bring DVD’s and magazines like National Geographic for the exchange. During this action about 150 books were exchanged, and the remaining books were saved for the next exchange. Due to a lower interest of RBI employees for this event, the Library has decided to prolong the period between two exchanges.

EDUCATION

Members of Library staff were involved in undergraduate and graduate level teaching at the University of Zagreb and University of Zadar.



Figure 3: Library presentation point at RBI Open Days 2013

PROJECTS

Research, developmental and international projects

1. 2nd Generation of Open Access Infrastructure for Research in Europe - OpenAIREplus, Jadranka Stojanovski, FP7, Grant agreement number: 283595
2. Support for Establishment of National/Regional Social Sciences Data Archives - SERSCIDA, Alen Vodopijevic (associate), FP7



Figure 4: Library's FP7 projects - OpenAIREplus and SERSCIDA

SELECTED LECTURES

1. Macan B. Open access repositories – interoperability as the only way. 13th round table on free access to information: publishers and libraries, Zagreb, December 10, 2013.
2. Pehar F, Stojanovski J. Science beyond PDF. Science Festival, Zagreb, Croatia, April 22-28, 2013.
3. Macan B, Vodopijevec A. Open the access to information. 108. Colloquium of Ruđer Bošković Institute Library, Zagreb, Croatia, October 10, 2013.

SELECTED PUBLICATIONS

1. Macan B, Fernández GV, Stojanovski J. Open source solutions for libraries: ABCD vs. Koha. *Program-electron Lib* **47** (2013) 136.
2. Frančula N, Lapaine M, Stojanovski J. Selection of non mapping sciences journals suitable for publishing mapping sciences topics. *Geod List* **67** (2013) 271.
3. Frančula N, Stojanovski J, Lapaine M. Defining the Corpus of Mapping Sciences Journals. *Kartografija i geoinformacije* **12** (2013) 4.
4. Pažur I. Presence of e-book in academic and related libraries in Croatia. *Vjesnik bibliotekara Hrvatske* **56** (2013) 171.
5. Pažur I. Library of the Ruđer Bošković Institute on social networks // 12th round table on free access to information “social networks and libraries”. Barbarić A, Mučnjak D, (eds.). Zagreb, *Hrvatsko knjižničarsko društvo*, 2013, pp 92-109.

Notes

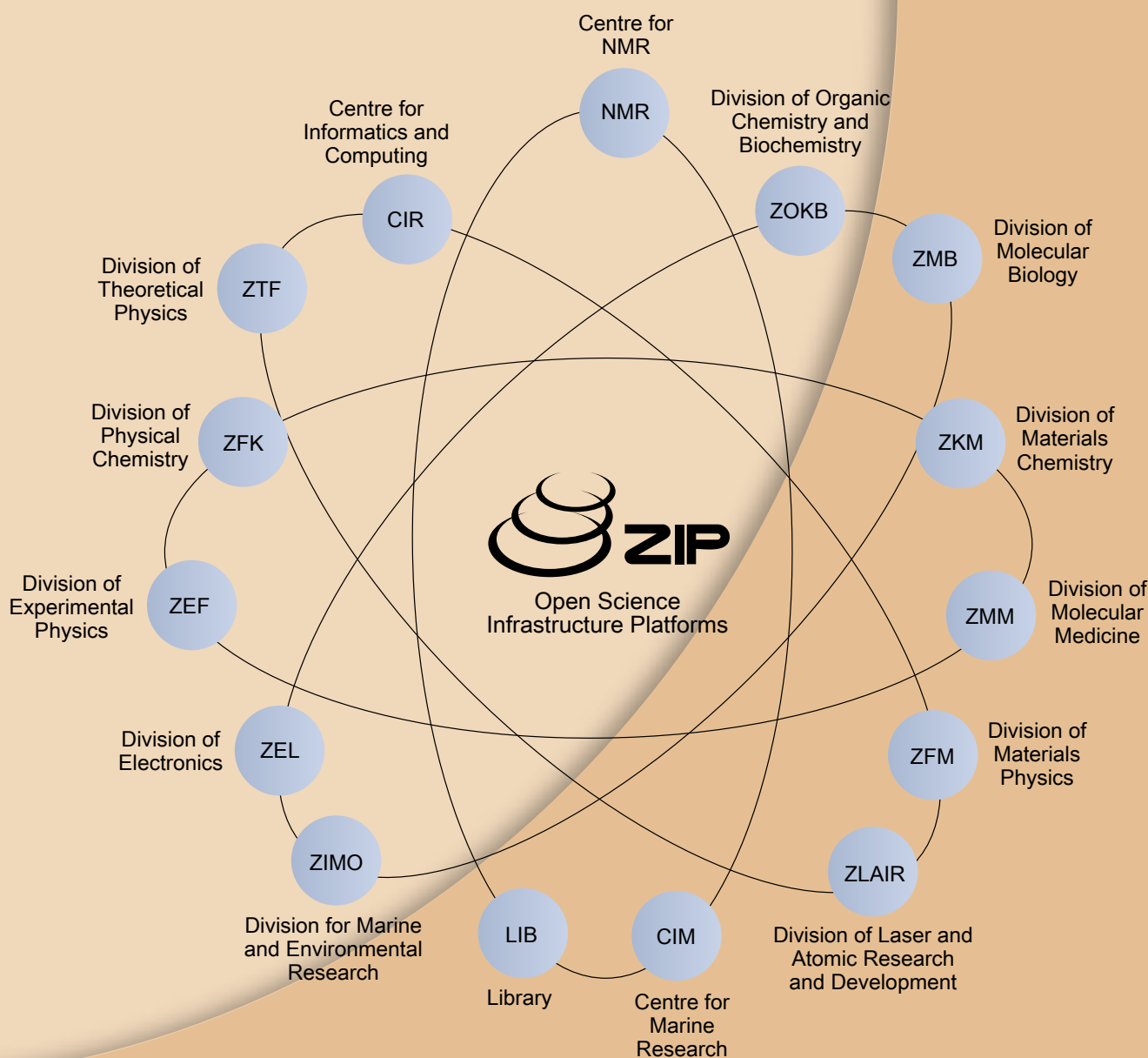




Nikola Tesla
1856 - 1943



Ruđer Bošković
1711 - 1787



The Ruđer Bošković Institute is the largest Croatian research centre dedicated to fundamental and applied science research. More than 500 academic staff and graduate students work on an array of scientific problems in a multi-disciplinary environment. In Croatia, the RBI is the premiere national institution dedicated to research, higher education and the provision of scientific and technical support to academia, state and local governments and technology based industries. The RBI is part of the EU European Research Area and participates in numerous international collaborations with research institutes and universities sharing the same values and vision.