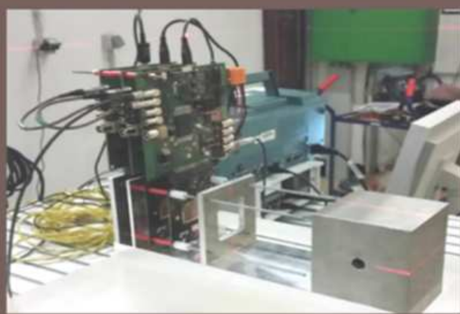
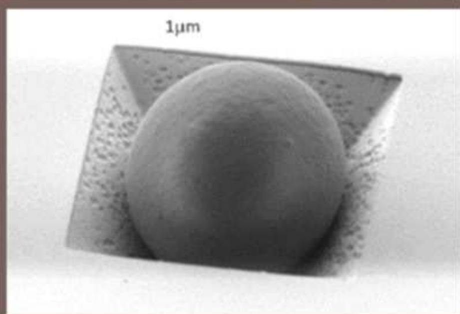
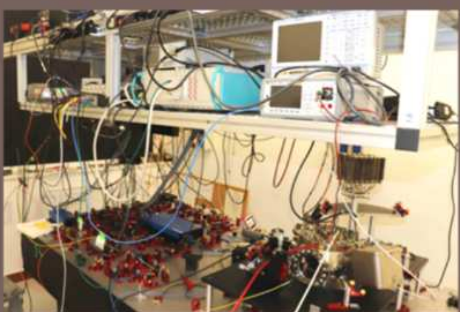
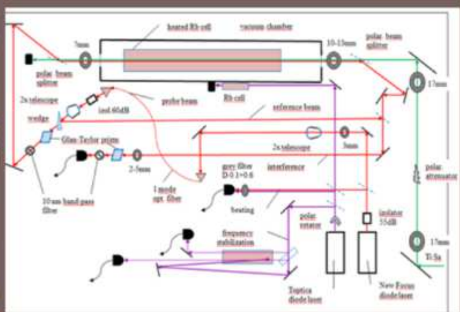
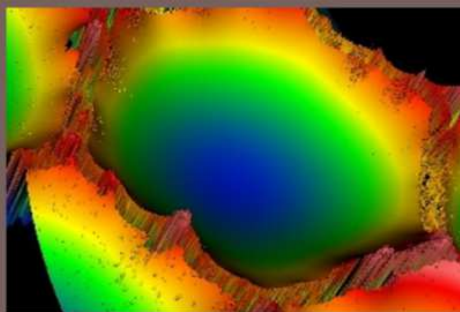
2018











Wigner Research Centre for Physics
Hungarian Academy of Sciences
Budapest, Hungary

Wigner RCP 2018

Annual Report

Wigner Research Centre for Physics
Hungarian Academy of Sciences
Budapest, Hungary
2019

Wigner Research Centre for Physics

Hungarian Academy of Sciences

Budapest, Hungary

2019

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Hungarian Academy of Sciences

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Wigner RCP 2018 – Annual Report

Edited by T.S. Biró, V. Kozma-Blázsik, B. Selmeci

Proofreader: I. Bakonyi

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FOREWORD

from the Director of the Institute for Solid State Physics and Optics

It is my privilege to present, for the final time before my retirement, the 26th edition of the Annual Report of the Institute for Solid State Physics and Optics of the Wigner Research Centre for Physics. During my career at the Institute spanning 41 years we underwent two restructurings. The first in 1992, when the well-known Central Research Institute for Physics of the Hungarian Academy of Sciences (KFKI) was split into four independent institutions, followed by the second in 2011, when our institute merged with the Institute for Particle and Nuclear Physics, to form the Wigner Research Centre for Physics. Over the last four decades much has changed: the Soviet Bloc collapsed, our social and economic system changed, and travel without restrictions became possible. It was an exciting era when the world opened and expanded around us. During this transition period it was a great challenge, with my colleagues, to overcome all the new obstacles. This made our lives vibrant, colourful, and adventurous.

I am pleased to announce that 2018 was yet another successful year for the Institute of Solid State Physics and Optics. In today's world, competitiveness of a nation and success of a society is increasingly determined by its human potential: its well-educated and creative members abounding with ideas and readiness to make a contribution (in Count István Széchenyi's rather freely translated words). This is even more pronounced in scientific research and development where new insights and inventiveness play crucial roles.

The core mission of management is to maintain the necessary environment in which our research groups can prosper and achieve outstanding scientific results. Regardless of the new plans for yet another reorganization that has gained traction over the past mouths, our staff remains motivated, our scientists continue to work assiduously, and their considerable efforts have earned significant recognition from both our local scientific community and from a much wider national and international audience. One colleague received the Széchenyi Prize, a major award by the state recognizing outstanding contributions to academic life in Hungary. The activities of all four Lendület (Momentum) Research Groups exceeded expectations. The leader of the Strongly Correlated Systems group won the Humboldt Research Award. A young scientist from the Semiconductor Nanostructures Lendület Group received the Young Investigator Finalist Award for his research, while PhD students and postdocs received Scholarships from the Ministry of Human Resources a Tempus Mundi Internship and membership of the Premium Postdoc Program of HAS. The Ultrafast, high intensity light-matter interactions Lendület Group is a Max Planck Partner Group. Last but not least, the Quantum Optics Lendület Group became the consortium leader of the more than 1 million Euro HunQuTech project. The institute currently has another four outstanding groups, the Wigner Research Groups, which we hope will grow to become future Lendület groups or project leaders. It has become a tradition at the institute to award prizes for outstanding publication activity as well as for applied research. This year an ambitious PhD student from the Semiconductor Nanostructures Lendület Group won this prize based on his high impact factor articles, notably published in Nano Letters and Nature Communications.

The present yearbook highlights our activities and presents the organization that we have developed throughout the years. We briefly summarize our 2018 scientific activities and the achievements of our 20 research groups. For this purpose, we list selected publications, grants and contracts, as well as applications and related academic and outreach activities.

Of the total of 204 papers authored by our researchers in 2018, approximately two-thirds have foreign co-authors, highlighting our colleagues' strong ties with researchers in over 30 countries, primarily in the European Union, but also in many other international universities and research institutions. The institute interacts with 45 foreign universities and institutions, among which 18 are German, 8 American and 4 Japanese. Among the 18 research institutions with whom we collaborate 15 are in the EU and associated countries and one in each of Australia, Egypt and Japan.

Our scientists' achievements are acknowledged through a number of international contracts and collaborations such as the H2020 RI projects including BrightnESS and IPERION-CH, the FET Open projects such as NEURAM and Petahertz Opt. Com, VISGEN as our first MSCA Rise project and collaborations like ASTERIQs. In the field of quantum technology there is the HunQuTech consortium led by our institute and two additional Quant ERA projects. The V4-Korean, the Japanese-Hungarian collaboration programs, and the two NKP and KKP National Excellence Programs are among the most significant.

Such accomplishments play a key role in keeping excellent researchers at our institute in spite of the strong brain drain, not only to more scientifically developed countries, but increasingly to local industry. Competitiveness and success can only be achieved by bolstering human potential. Our priority challenge is to provide a modern scientific infrastructure in an inspiring intellectual environment to attract and retain the most talented students and young researchers.

I hope this booklet will provide you with useful information regarding the development of the institute and its main achievements in the fields of quantum optics, solid state physics, laser physics, applied and nonlinear optics, complex fluids, neutron spectroscopy and a number of applications – e.g. in environmental science, biology, pharmacology, toxicology, medicine, etc.

This publication is directed not only at the scientific community, but to all interested readers in Hungary and abroad who would like to catch a glimpse of the activity of our institute as witness to milestones in the history of Hungarian science.

Aladár Czitrovszky

director of the Institute for Solid State Physics and Optics

of the Wigner Research Centre for Physics

AWARDS AND PRIZES

Awards of the State of Hungary and Government of Hungary

L. Gránásy, Széchenyi award

Awards of the Hungarian Academy of Sciences

L. Szabados: Physics Prize of the Hungarian Academy of Sciences
K. Szegő: Eötvös József Wreath Award of the HAS
T. Pusztai: Prize of the HAS

International professional awards

T. Csörgő (representing TOTEM-Hungary): TOTEM 2018 Achievement Award, by the Spokesperson and the Chair of the Collaboration Board, TOTEM Collaboration
F. Nemes: TOTEM 2018 Publication Award, by the Spokesperson and the Chair of the Collaboration Board, TOTEM Collaboration
D. Kincses: Fulbright Student Award (US-Hungarian Fulbright Foundation for Educational Exchange) to SUNY Stony Brook (Prof. Roy A. Lacey, supervisor)
M. Varga-Kőfaragó: ALICE thesis award
L. Földy, NASA Group Achievement Award to Cassini Plasma Spectrometer Team
Sándor Szalai and the Space Technology Group: NASA Aeronoutics and Space Administration Group Achievement Award to Cassini Spectrometer team
P. Érdi, Florence J. Lucasse Fellowship for Excellence in Scholarship.
Ö. Legeza: Humboldt Research Award
V. Ivády: Among the five finalist Psi-k Volker Heine Young Investigator Award, 2018
A. Czitrovszky: honorary member of the Ukraine Academy of Sciences and Education

National professional awards

R. Kovács: Györgyi Géza Prize of the Wigner RCP of the HAS 2018
M. Varga-Kőfaragó: Wigner RMI Directors praise
A. Opitz: ELFT Jánossy Lajos Award.
G. Thiering: Publication Award of the Wigner RCP SZFI
G. Thiering: György Ferenczi Memorial Award
A. Derzsi: ELFT Schmid Rezső Award 2018

Bolyai János Scholarship of the HAS granted in 2018

G. Barcza	Sz. Szalay	L. Temleitner	Sz. Pothoczki
B. Mikóczi	P. Kovács	D. Nagy	A. Vukics

New National Excellence Program (ÚNKP) scholarships

B. File	M.A. Pocsai	Sz. Szalay	D. Beke
A. Csóré	L. Kocsor	É. Tichy-Rács	N. Kiss

Other scholarships

B. File: EFOP-3.6.3-VEKOP-16-2017-00002, Non-conventional computational and modelling approaches (PPKE-ITK)

Á. Gali: KKP Élvonal (Excellence Grant), NKFIH Grant No. 129886

V. Ivády: Premium Postdoctoral Programme of the HAS

A. Csóré: Tempus Mundi Internship

N. Kiss:International Investigative Dermatology International Trainee Retreat scholarship, Orlando, FL

Other awards

D. Kincses: SCIndicator of the Year prize (SCIndikátor science-communication quiz)

D. Kincses: Audience Award (SCIndikátor science-communication quiz)

Oláh László, Balogh Szabolcs József, Hamar Gergõ, Varga Dezsõ, Gera Ádám László, Nyitrai Gábor, Pázmándi Zsolt: Award of Excellence, Fizikai Szemle

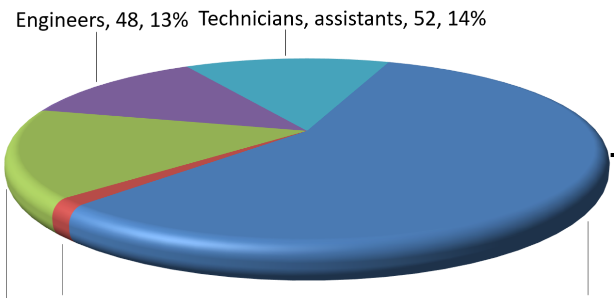
G. Thiering: Publication prize (1st) of the Department of Atomic Physics, BME

N. Kiss:Semmelweis University Excellent Management of Undergraduate Students award.

N. Kiss:Trialect for Non-Invasive Diagnostic, Surgical, and Cosmetic Dermatology Fellowship, Rome.

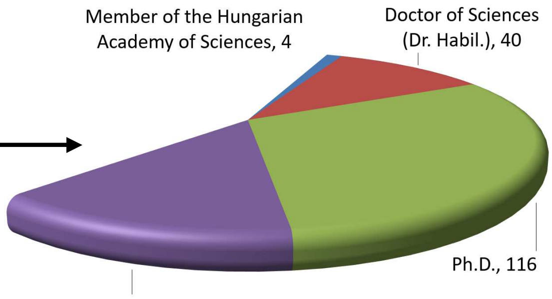
Permanent staff by profession

Total: 376



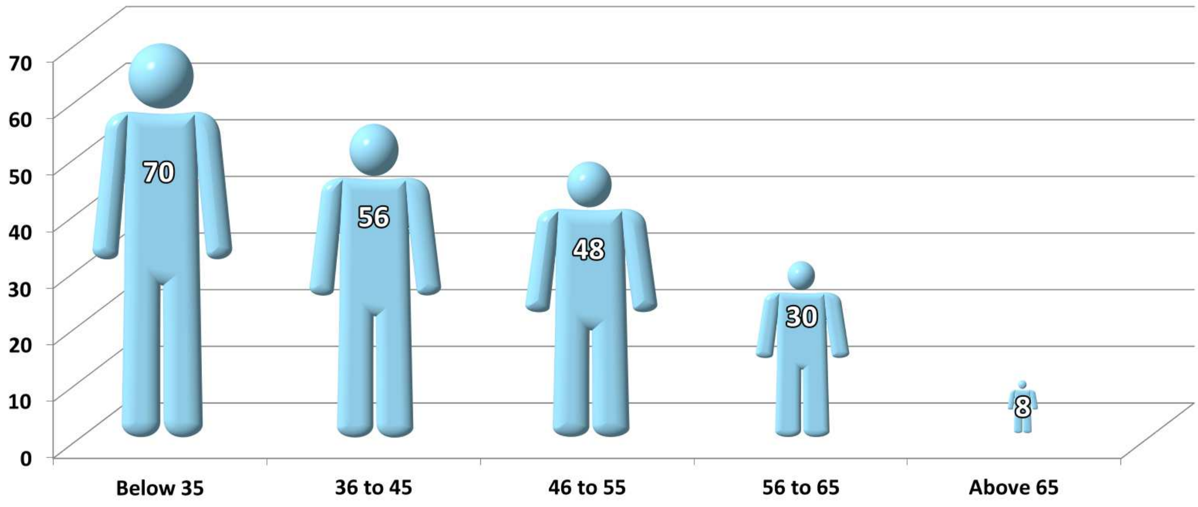
Scientists by degree/title

Total: 212

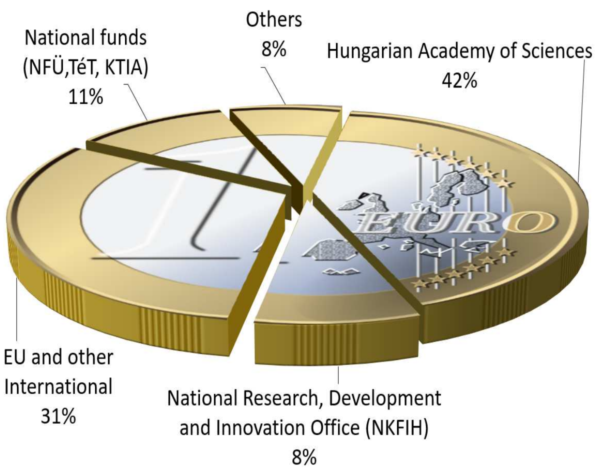


Scientists by age group

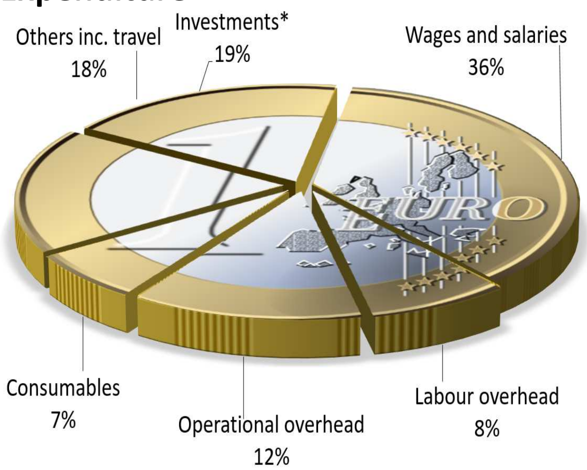
Total: 212



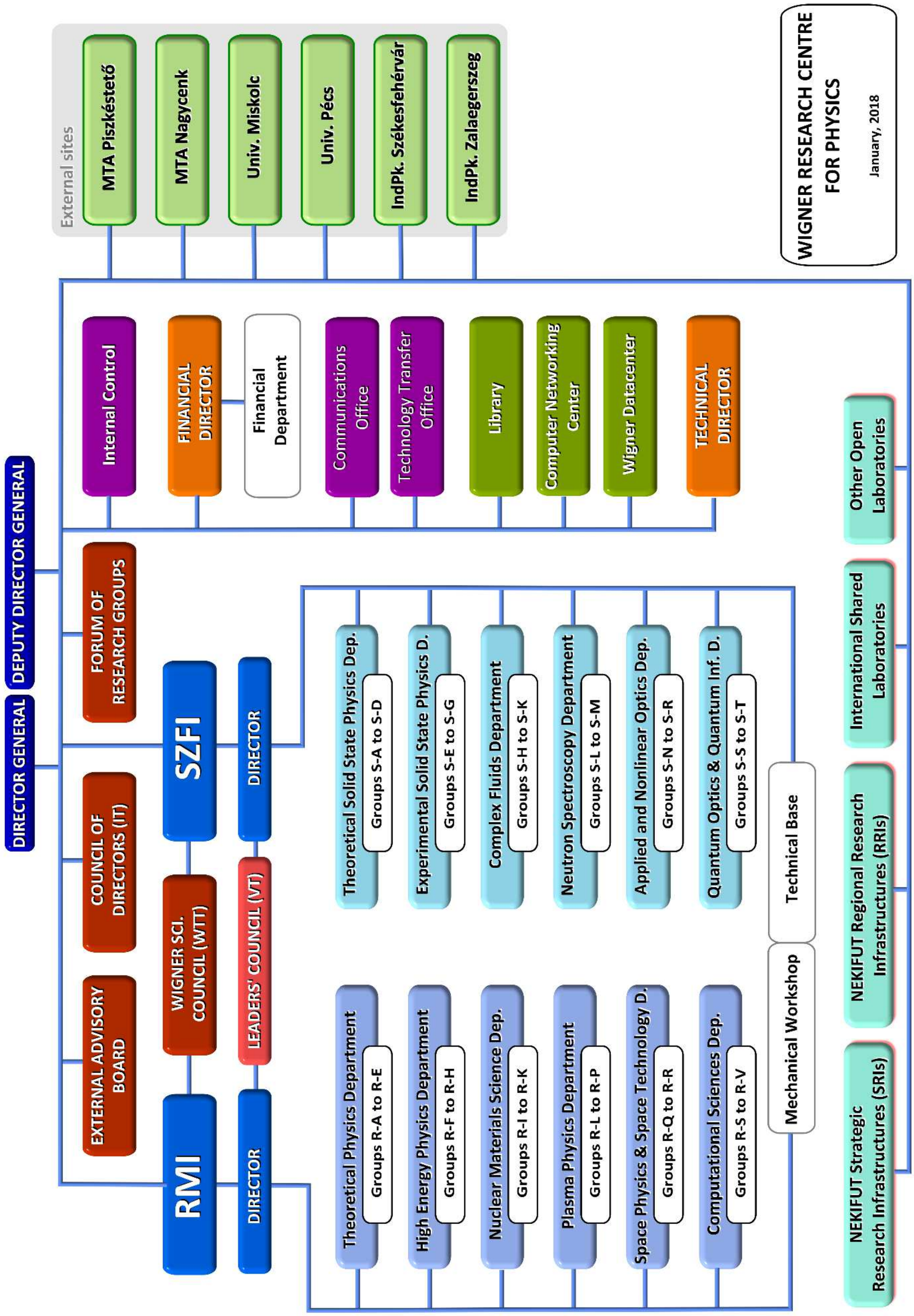
Income*



Expenditure*

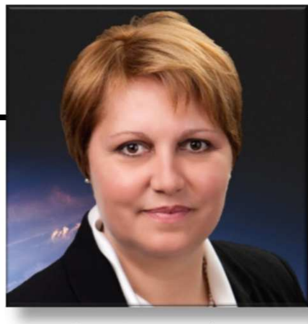


*V.A.T not included.



DIRECTOR GENERAL
DEPUTY DIRECTOR GENERAL
EXTERNAL ADVISORY BOARD
COUNCIL OF DIRECTORS (IT)
FORUM OF RESEARCH GROUPS
RMI
WIGNER SCI. COUNCIL (WTT)
SZFI
DIRECTOR
LEADERS' COUNCIL (VT)
DIRECTOR
Theoretical Physics Department
Groups R-A to R-E
High Energy Physics Department
Groups R-F to R-H
Nuclear Materials Science Dep.
Groups R-I to R-K
Plasma Physics Department
Groups R-L to R-P
Space Physics & Space Technology D.
Groups R-Q to R-R
Computational Sciences Dep.
Groups R-S to R-V
Theoretical Solid State Physics Dep.
Groups S-A to S-D
Experimental Solid State Physics D.
Groups S-E to S-G
Complex Fluids Department
Groups S-H to S-K
Neutron Spectroscopy Department
Groups S-L to S-M
Applied and Nonlinear Optics Dep.
Groups S-N to S-R
Quantum Optics & Quantum Inf. D.
Groups S-S to S-T
Mechanical Workshop
Technical Base
Internal Control
FINANCIAL DIRECTOR
Financial Department
Communications Office
Technology Transfer Office
Library
Computer Networking Center
Wigner Datacenter
TECHNICAL DIRECTOR
External sites
MTA Piszkéstető
MTA Nagycenk
Univ. Miskolc
Univ. Pécs
IndPk. Székesfehérvár
IndPk. Zalaegerszeg
NEKIFUT Strategic Research Infrastructures (SRIs)
NEKIFUT Regional Research Infrastructures (RRIs)
International Shared Laboratories
Other Open Laboratories
WIGNER RESEARCH CENTRE FOR PHYSICS
January, 2018

WIGNER AND ESA TECHNOLOGY TRANSFER PROGRAM



Zsuzsanna Tandi – Innovation Adviser and Head of the European Space Agency 'National Technology Transfer Initiative in Hungary' and ESA Business Incubation Centre Hungary

In 2013, Wigner Research Centre for Physics of the Hungarian Academy of Sciences (Wigner RCP HAS) established the position of Secretary of Innovation to promote the industrial exploitation of the results generated during the researches. The Wigner RCP HAS has developed its Intellectual Property Right Rules and the administrative background pursuant to the regulations of the Headquarters of the Hungarian Academy of Sciences and the current laws.

The management have attended numerous events and conferences, which provided opportunities to meet industrial partners, demonstrate the Institute's capabilities, and the potentials of a cooperation with MTA Wigner RCP. The research teams of the Institute have successfully completed industrial orders.

In 2016, we established our Technology Transfer Office in association with the European Space Agency (ESA). Since December 6, 2016, the office has been operating the "*National Technology Transfer Initiative in Hungary*" (NTTI) programme with the approval of the Ministry of National Development and ESA. The programme made it possible for the Office to expand to 7 people (3 persons in full time and 4 in part time).

esa business incubation centre Hungary

As a result of the successful implementation of the ESA NTTI programme, the second pillar of the ESA Technology Transfer Programme has also opened up for Hungary. ESA and the Ministry of National Development (later the Ministry of Foreign Affairs and Trade) repeatedly selected the Wigner RCP HAS as a partner to implement the second pillar in Hungary. Signing the contract on June 27, 2018, we were granted the right to open the Business Incubation Centre (BIC) of ESA as a joint programme of the Hungarian Academy of Sciences and ESA. The incubator programme was launched on July 2, 2018.

Opening ceremony of the ESA Business Incubation Centre Hungary: Martin Kern, EIT interim director; Levente Magyar, Deputy Minister of Foreign Affairs and Trade; Johann-Dietrich Wörner, ESA Director General; Zsuzsanna Tandi, Head of ESA BIC Hungary; Ádám Török, F.M., Secretary-General of HAS, Péter József Lévai, Director General of Wigner RCP HAS

The Business Incubator and the NTTI operate with the same staff and at the same location. This merger of the two programmes, which was also an innovation within the ESA network, are working successfully in synergy, earning a strong reputation among the other 20 international ESA offices.

Since 2013, the Secretary of Innovation is also a member of the HEPTech project at CERN (High Energy Physics Technology Transfer Project). In May 2017, she was also invited to the ARIES (Accelerator Research and Innovation for European Science and Society). These steps deemed necessary for the professional handling of intellectual property generated by the research institute. Being a part of these institutions, we acquired refined protocols, well-functioning frameworks that is of great help during the implementation of the ESA Technology Transfer Program.

The Hungarian ESA 'National Technology Transfer Initiative' office is one of the 4 priority ESA offices. The Office has its own source of applications, and provides support for demonstration projects. The Hungarian Office supports continuously many technology transfer projects and financially supports 2 projects per year as grants.

The research teams will have the opportunity to communicate with industrial partners of the Incubator program. They can receive continuous feedbacks in relation to their research. In addition, maintaining live connection they can get investor resources. Thanks to the infrastructural support of the Hungarian Academy of Sciences, the Incubation Centre was given the opportunity to operate in a fully renovated and equipped, almost 450 m^2 modern environment at the KFKI campus, which is open to the researchers of the Hungarian Academy of Sciences.

Training room of ESA BIC Hugary

Corridor of ESA BIC Hungary

Our objective is to contribute to the economic development of Hungary, strengthen businesses, create jobs, and help to launch new ventures. In addition, our network encourages Hungarian entrepreneurs to launch businesses abroad.

esa space solutions

ESA Business Incubation Centre Hungary has become the member of ESA BICs network providing support all over Europe. ESA BIC Hungary (and the ESA NTTI Hungary also) helps to transfer technology from space to non-space applications and will support 25 Hungarian start-ups over a 5-year period to develop products for terrestrial use. It executes the overall implementation and management, such as

- supporting start-ups during the incubation phase by providing accommodation, business and technical support and coordination,

- identifying Financial Partners to provide access to finance, loan schemes or seed equity funds;
- supporting the selected applicants during the execution of the activities in order to achieve meaningful results;
- organising events and training

Presswall of ESA BIC Hungary

INTERNATIONAL SCIENTIFIC COOPERATION

Valéria Kozma-Blázsik, scientific secretary

Every year ushers in new scientific and societal advancements, challenged by new risks and threats, steadily raising the expectations placed by society. Scientific research is an area of constant change and progress that requires great flexibility from its participants to adapt quickly to a continuously evolving environment. The year 2018 started like a typical year; scientists continued with their research, published new articles, carried out experiments, developed and built new equipment to implement their project goals. Thanks to their great energy and motivation, 2018 turned out to be yet another success.

As in previous years, Wigner's research teams continued to harness their strengths, publishing in high ranking scientific journals, actively participating in the Hungarian higher education system, and tirelessly writing grant proposals to expand their horizons and financial means.

Wigner's research groups cover a wide range of specialities within physics as reflected through their publications. In 2018, altogether 870 **scientific publications** were published by members of the two institutes. Of these 651 articles from RMI, a great proportion in large collaborations mainly partnering with CERN, and 217 from SZFI in different topics of material sciences, photonics and quantum optics.

The largest portion of the articles are the result of collaborative projects. This year researchers participated in around 75 **projects,** among them 13 EU, 6 non-EU but internationally funded such as ESA, NIH etc., and 53 national projects of various kinds with grant amounts above 5 million HUF (about €15.000), in addition to about 30 smaller mobility projects. Researchers took part in 20 consortia with international and Hungarian partners, mainly from universities and other research institutes. Finally, there were a dozen long-term and a handful of new collaborations with industrial partners.

We mention the applications of cosmic muons for large-scale imaging among the successful research directions at the Institute of Particle- and Nuclear Physics in recent years. An important application of cosmic muons detectors was developed for the imaging interiors of volcanos. The Japanese NEC company licensed our muography observation system (MOS) for research purposes, and extended its licensing rights and committed funding for the coming year. During the term 2017 - 2021 the Institute of Solid State Physics and Optics is acting as coordinator of the HunQuTech Consortium in the framework of the National Excellence Program 2017 on Quantum Technology with a budget of 3,5 billion HUF. This year alone the research centre administered 3,1 billion HUF of project revenue (approx. 9,8 M €).

Researchers of the Wigner Research Centre are very active in Hungarian **academic education** and the Doctoral Schools. They continuously build strong ties with their many university students, mentoring them during their Masters theses, TDK projects, and PhD degrees.

However, during the last few years we had to address a new set of challenges including high turnover rates mainly among our young scientists. From year to year it is increasingly difficult to attract young talent. To counter this process on the long term, we increasingly focus on outreach activities towards the high school generation, and organize events such as Open Days, and Girls' Day to awaken early interest in scientific careers. In 2018, we organised our first five-day Summer Camp for 10 students, during which they carried out a small project at the 5 participating laboratories. Motivated by the success of this initiative we plan to repeat it in the framework of a longer 10-day program, which would enable students to gain deeper insights to their topic of choice. It was also the first year that we offered internships to students studying at UK universities. We hope that providing them with a first-hand working experience at our institutes will offer them a long term alternative to leaving the country.

Our research centre must compete not only with the allure of research possibilities abroad, but also with the strong financial incentives offered by industry. If this now one-way mobility into industry would be flowing equally in both directions, it would be present young researchers with invaluable means for gaining experience. Our MSCA Visgen RISE project is setting the example for this new type of academia-industry bidirectional relationship.

In the first 6-7 months of the year business was as usual, but by mid-year we were faced with the possibility of yet another reorganisation, the second since 2012, when the Wigner Research Centre for Physics was founded. Since then we have made considerable steps to create a fresh organisational culture, building on the strength of the two merging research institutes of the former KFKI campus. We owe thanks to a few significant national VEKOP projects awarded in the last two years that provided the financial means to catalyse this process. Based on this revenue we could build and strengthen interdepartmental and interdisciplinary cooperation with 'Lendület'- Momentum groups from both institutes RMI and SZFI working together on Ultrafast experiments for better functional molecules, nanocircuits, and atomic beams.

For the past 11 years, I have been working for Wigner and its predecessor institute. I am witness to the new developments of a continuously evolving ecosystem. We do our best to find novel ways to introduce new innovative ideas and transform to achieve our goal of becoming a true learning organisation.

Once again, we can conclude that the significant achievements of Wigner during the past year reflect the hard work of our people and our commitment to make a difference through:

Looking outwards to listen and respond to society, engage constructively with academic professionals, government, and industry;

Looking forwards to respond effectively to emerging challenges, benefiting from emerging knowledge and technologies; and

Looking after our people and the resources entrusted to us in order to search for and give scientific answers to pressing issues of our contemporary world.

OUTSTANDING RESEARCH GROUPS*

MTA’s “Momentum” Research Teams

The goal of the “Momentum” Program of the Hungarian Academy of Sciences (HAS) is to renew and replenish the research teams of the Academy and participating universities by attracting outstanding young researchers back to Hungary. The impact and success of this application model is highly acclaimed and recognised by the international scientific community. Initiated by the former HAS President József Pálinkás, the “Momentum” Program aims to motivate young researchers to stay in Hungary, provides a new supply of talented researchers, extends career possibilities, and increases the competitiveness of HAS' research institutes and participating universities.

Wigner Research Groups

The “Wigner Research Group” program is introduced to provide the best 3-3 research groups from both institutions of the Centre with extra support for a year. Its primary goal is to retain in science and in the Research Centre those excellent young researchers who are capable of leading independent research groups. It aims to energize research groups, and to recognize, support and raise the profile of the leader of the group. During the support period the research group should make documented efforts to perform successfully on domestic R&D tenders and international tenders of the EU and its member states.

* **Abbreviations in the researcher lists of the scientific projects:**

#: PhD student

A: associate fellow

E: professor emeritus

R-A. Field theory

Wigner Research Group

Zoltán Zimborás, Gabriella Böhm, Viktor Czinner[A], László Fehér, Gyula Fodor, Péter Forgács, Gyula Kluge[A], Zoltán Kunszt[A], Árpád Lukács, Balázs Mikóczi, Júlia Nyíri[A], László B. Szabados, Kornél Szlachányi, Kálmán Tóth[A], Gábor Zsolt Tóth, Péter Vecsernyés

Einstein-conformally coupled Standard Model. — We introduced and studied a classical field theoretical model, the so-called Einstein-conformally coupled Standard Model (EccSM), which is general relativistic and in which (according to the key idea above) the matter sector is coupled to gravity in a conformally invariant manner. We showed that, in this theory, in addition to the usual initial Big Bang singularity there might be a so-called Small Bang singularity, too (in which it is only the spacetime geometry is singular but all the matter field variables remain bounded), and that in the generic case Newton's gravitational constant yields an absolute upper bound for the magnitude of the Higgs field. Furthermore, the resulting rest masses of the fields depend on time, and although their time dependence can be neglected soon after their genesis, but about 10^{-27} seconds after the initial singularity (which is the characteristic time of the weak interactions) this time dependence could still in principle be shown up in the starting up particle physics processes.

Noether currents for the Teukolsky master equation. — The Teukolsky master equation is an important wave equation that governs the evolution of the extreme spin weight components of the electromagnetic, linearized gravitational, neutrino and spin-3/2 fields in Kerr (i.e., rotating black hole) spacetime. For various purposes, e.g. for testing numerical simulations and for studying the decay properties of the mentioned fields, it is desirable to know conserved currents for this equation. However, the Teukolsky master equation does not follow from a Lagrangian, therefore the usual procedure, which is to apply Noether's theorem, is not suitable for finding conserved currents for it. By applying a less well-known variant of Noether's theorem, we showed that a pair of Teukolsky master equations with opposite spin weights does follow from a Lagrangian, and constructed conserved currents that correspond to the time translation and axial symmetries of the Kerr spacetime and to the scaling symmetry of the Teukolsky master equation. These currents involve two independent solutions of the Teukolsky master equation with opposite spin weights. We also introduced general definitions for the symmetries and conserved currents of boundary conditions of partial differential equations, extended Noether's theorem and its variant to them, and used this extension of the latter variant to construct conserved currents associated with the Sommerfeld boundary condition in the case of the Teukolsky master equation. Such boundary conserved currents are again useful for testing purposes in numerical simulations.

Quantum Correlations in Many-Body Systems. — We studied various types of quantum correlations in many-body systems and field theories. One of these was entanglement negativity, which is a versatile measure of entanglement that has numerous applications in quantum information and in condensed matter theory. It can not only efficiently be computed in the Hilbert space dimension, but for Gaussian bosonic systems, one can compute the negativity efficiently in the number of modes. However, such an efficient computation does

[A] Associate fellow

not carry over to the fermionic realm, the ultimate reason for this being that the partial transpose of a fermionic Gaussian state is no longer Gaussian. To provide a remedy for this state of affairs, we introduced efficiently computable and rigorous upper and lower bounds to the negativity, making use of techniques of semi-definite programming, building upon the Lagrangian formulation of fermionic linear optics, and exploiting suitable products of Gaussian operators. We also discussed examples in quantum many-body theory with applications in the study of topological properties at finite temperature.

Another investigated measure was the quantum Fisher information. We calculated the Fisher information quantity for different states of atomic ensembles in a magnetic field, see Fig. 1. The value of the Fisher information can signal nonclassicality, but it is also important from a metrological point of view. In particular we calculated precision bounds for estimating the gradient of the magnetic field based on the quantum Fisher information. We also considered a single atomic ensemble with an arbitrary density profile, where the atoms cannot be addressed individually, and which is a very relevant case for experiments.

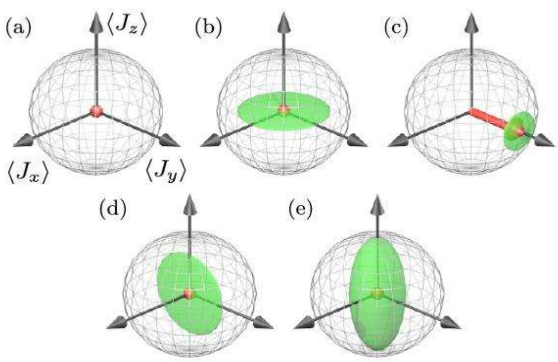


Figure 1. *Angular momentum components and their variances for various spin states for few particles are shown: (a) singlet state, (b) z-Dicke state, (c) state totally polarized in the y-direction, (d) x-Dicke state, (e) GHZ state.*

Grants

OTKA[1] MAT K 124138 "Crossed modules over Hopf monoids" (G. Böhm, 2017-2021)

OTKA K111697 "Group-theoretic aspects of integrable systems and their dualities" (L. Fehér, 2014-2018)

OTKA PD 116892 "Highly eccentric signals in gravitational wave physics"(B. Mikóczi, 2015-2018)

International cooperations

Departamento de Álgebra and CITIC, Universidad de Granada, Spain

Department of Mathematics, Macquarie University, Sydney, Australia

Paris Observatory, Meudon, France

Université de Tours, France

Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Germany

[1] OTKA: National Scientific Research Fund

Institute of Theoretical Physics and Astrophysics, Faculty of Mathematics, Physics and Informatics, University of Gdansk, Poland

Publications

Articles

1. Böhm G, Gomez-Torrecillas J, Lack S: Weak multiplier bimonoids. ***APPL CATEGOR STRUCT*** **26**:1 47-111 (2018)
2. Eisert J, Eisler V, Zimborás Z: Entanglement negativity bounds for fermionic Gaussian states. ***PHYS REV B*** **97**:16 165123/1-12 (2018)
3. Fodor G: Localized objects formed by self-trapped gravitational waves. ***ASTRON REP+*** **62**:12 874-881 (2018)
4. Szabados LB, Wolf G: Singularities in Einstein-conformally coupled Higgs cosmological models. ***GEN RELATIV GRAVIT*** **50**:10 136/1-34 (2018)
5. Szabados LB: On gravity's role in the genesis of rest masses of classical fields. ***GEN RELATIV GRAVIT*** **50**:3 Paper: 34 , 21 p. (2018)
6. Apellaniz I, Urizar-Lanz I, Zimborás Z, Hyllus P, Tóth G: Precision bounds for gradient magnetometry with atomic ensembles. ***PHYS REV A*** **97**:5 053603/1-17 (2018)

Book chapter

7. Böhm G: *Hopf algebras and their generalizations from a category theoretical point of view*. Lecture Notes in Mathematics, Springer Nature Switzerland AG (2018), pp. 1-165

Other

8. Fehér, L: Poisson-Lie analogues of spin Sutherland models (2018) https://arxiv.org/abs/1809.01529
9. Szabados LB: A gravitációs energia-impulzusról (On gravitational energy-momentum, in Hungarian). ***FIZIKAI SZEMLE*** **68**:6 183-188 (2018)

See also: R-B.7, R-G.2, S-B.5, S-S.1

R-B. Heavy-ion physics

Wigner Research Group

Gergely Gábor Barnaföldi, Gergő Almássy, Gábor Balassa, Gyula Bencze[A], Dániel Berényi[#], Gábor Bíró[#], Tamás Sándor Biró, Pál Doleschal[A], Edit Fenyvesi[#], Vahtang Gogohia[A], Miklós Gyulassy[A], Miklós Horváth, Szilvia Karsai[#], Péter Kovács, Róbert Kovács[#], Péter Lévai, Péter Pósfay[#], János Révai[A], K. Shen, Péter Ván, György Wolf, Miklós Zétényi, B. Zhang

High-energy heavy-ion physics is connected to a large variety of physics disciplines. Our researches probe fundamental concepts of classical and modern thermodynamics, hydrodynamics, and quantum theory. Therefore, we have several theoretical and practical topical research directions covering a wide spectrum, such as: thermodynamics, perturbative and non-perturbative Quantum Chromodynamics (QCD), high-energy nuclear effects, hadronization, hadron phenomenology, phenomenology of compact stars, and gravity/cosmology. Our studies are strongly motivated by the needs of several recent and planned largescale facilities, such as collaborations at the LHC (CERN, Switzerland) and RHIC (BNL, USA), and future experiments at FAIR (GSI, Germany) and NICA (Dubna, Russia). We have continued our theoretical investigations in the direction of high-energy physics phenomenology connected to existing and future state-of-the-art detectors. Concerning international theoretical collaborations, we have established joint work with the Goethe Institute (Germany), LBNL (USA), CCNU, MAP (China), UNAM (Mexico), and ERI (Japan). We highlight below some of our major published results in details.

New developments in the effective field theory of the strong interaction. — As a member of the CBM collaboration, we continued the planning of the details of the detector. We participated in the detector simulations concentrated on the phi meson and on the double strange hypernuclei. We studied the physics cases as well.

We proposed a model based on the Statistical Bootstrap approach to estimate the cross sections of different hadronic reactions up to a few GeV in center of mass energy. The method is based on the idea, when two particles collide a so called fireball is formed, which after a short time period decays statistically into a specific final state. We used in a transport model for unknown cross sections.

We studied the masses of the low-lying charmonium states, namely, the J/Ψ, $\Psi(3686)$, and $\Psi(3770)$ in antiproton induced reactions. The masses of these states are shifted downwards due to the second order Stark effect. Using our transport model we showed that the in-medium mass shift can be observed in the di-lepton spectrum. Therefore, by observing the di-leptonic decay channel of these low-lying charmonium states, especially for $\Psi(3686)$, thus one can gain information about the magnitude of the gluon condensate in nuclear matter. This measurement could be performed at the upcoming PANDA experiment at FAIR as we published.

We analyzed the Xi^- baryon production in subthreshold proton-nucleus (p+A) collisions in the framework of our BUU type transport model. A new mechanism was proposed for Xi production in the collision of a secondary Lambda or Sigma hyperon and a nucleon from the target nucleus. It was found that the Xi^- multiplicity in p+A collisions is sensitive to the angular distribution of hyperon production in the primary N+N collision. Using reasonable assumptions on the unknown elementary cross sections we are able to reproduce the Xi^- multiplicity and the Xi^-/(Lambda+Sigma^0) ratio obtained in the HADES experiment.

In connection to cosmology, we studied the time evolution of the Einstein-conformally coupled Higgs cosmological models in the presence of Friedman–Robertson–Walker symmetries. We have found all the analytical singularities. We have shown that beyond the Big Bang singularity (singular curvature and diverging Higgs field there is another new kind of physical spacetime singularity (`Small Bang') where the curvature singular but the Higgs field is finite. Furthermore, we also have shown that there are nonanalytical singularities as well.

Multi-wavelenth astronomy investigations of superdense matter in compact stars.— Investigation of cold compact stars provides the opportunity to understand cold superdense matter and even, speculate on new states of matter. These theoretical developments are strongly connected to recent measurements of compact stars by multi-wavelength observations and gravitational waves. These projects are supported by theoretical networking EU COST action PHAROS (CA162014).

In collaboration with A. Jakovac (ELTE) we constructed a framework using the Functional Renormalization Group (FRG) technique for a one-fermion and one-boson theory with Yukawa-like coupling, where the equation of state (EoS) was calculated at finite chemical potential and zero temperature exactly – including quantum corrections. We investigated the effect of the quantum fluctuations on the nuclear equation of state and compact star observables. It was demonstrated, that correction to the mean field model can result 30% difference in the EoS, which modifies the neutron star mass and radius by 5% (see Fig 1). These interesting results were published in Phys Rev C and an extended study on the compactness in connection with multiwavelength astronomy measurements of GW170817 were published in PASA.

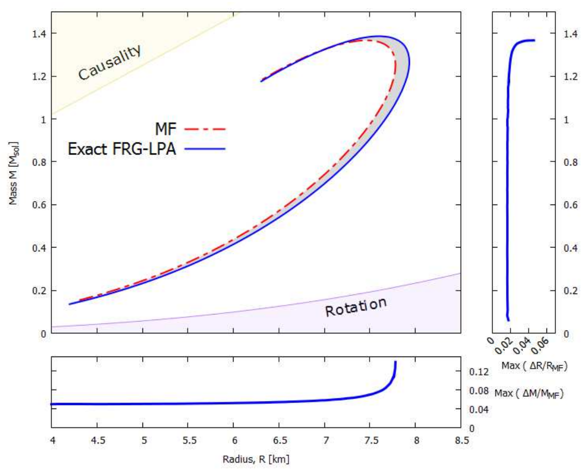


__Figure 1.__ Mass-radius diagram of the one-fermion and one-boson theory with Yukawa-like coupling, calculated in the mean field in and FRG framework. Relative difference of the two model is on the side graphs.

We started to investigate a realistic Waleckatype mean field model within this new framework. However an alternative gravitational theory, a Kaluza-Klein type compact object were also analyzed in a multifermion framework. This result has been presented on the IAU International Conference. In parallel, the foundations of continuum theories were further researched in non-relativistic, Galilean relativistic and special relativistic spacetimes.

Results from the non-extensive statistical approach. — High-energy heavy-ion collisions are good testbeds for the non-ideal, non-equilibrium, finite systems. The non-extensive statistical approach, developed by their group, can describe such a matter by enwidening the framework of classical thermodynamics and statistical physics towards non-equilibrium and complex system phenomena. This pioneering, novel approach to Tsallis, Renyi and further non-Boltzmannian entropy formulae have been applied by us in various physical phenomena from heavy-ion collisions, cosmology to networking.

We started a detailed study of the applied Tsallis–Pareto formulae. We found linear relations between the temperature parameter, T and the Tsallis parameter, q−1 , and the logarithmic dependence on the c.m. energy. The quark-hadron channels of the Tsallis–Pareto-like fragmentation functions were also fitted in electron-positron collisions. This result was quite promising, and presented similar values obtained from the fits of the hadron spectra in proton-proton collision. This fragmentation function parametrization was also tested in a direct pQCD calculation. Results were presented at The Hot Quarks Conference.

The entropy production during hadronization of the quark-gluon plasma was also investigated, based on the idea, that at high-energies the pair production and the number of resonances are increasing. We extended the original model with an energy dependent (non-linear) potential (non-constant string force) scenario. This predicts well the beam energy dependence of the total cross section.

The derivation of Cahn-Hilliard equation with Liu procedure clarifies the thermodynamic background of phase field theories and they opened a new approach of deriving them without any variational principles. We analysed the connection between mechanical and thermal continuum phenomena apply the thermodynamic methodology of internal variables and its consequences to develop new numerical methods, to model experimental results and for a comparison with other theories.

Phenomenology, transport, and hydrodynamics for heavy-ion collisions. — We investigated the emergence of the Chiral Magnetic Effect (CME) and the related anomalous current using the real time Dirac-Heisenberg-Wigner formalism. This method is widely used for describing strong field physics and QED vacuum tunneling phenomena as well as pair production in heavy-ion collisions. We investigated the strength of the CME in heavy ion collisions in the energy range of the SPS–RHIC–LHC accelerators, applying the Dirac–Heisenberg–Wigner formalism. The effect is strong and hopefully measurable at the $\sqrt{s}$ =10-60 GeV energy range, starts to become weaker at 130-200 GeV and disappears at LHC energies. Recent experimental data confirms these theoretical results. Final conclusion can be obtained after the analysis of the Beam Energy Scan data at the RHIC accelerator. This result has been published in Phys Lett B.

The dijet acoplanarity was investigated in heavy ion collisions. Nearly back-to-back di-jets with medium or large transverse momenta become acoplanar even in the vacuum due to multi-gluon radiation. This effect could become stronger in hot matter,generated in energetic heavy ion collisions. Thus the acoplanarity could carry information on the opacity of the hot matter. We described theoretically this dependence and made suggestions for experimental indications of modified acoplanarity. The analysis of recent LHC data may bring new insigth into the understanding of this effect and new data could help to determine the opacity in the real collisions. These result were presented at the Quark Matter 2018.

A further step was made in the theoretical model of the generalized Fourier-Navier-Stokes system in the framework of non-equilibrium thermodynamics. Solution methods for generalized heat conduction models, and analyzing our related experiments. The detailed analysis of the possible connections with kinetic theory.

In Boltzmann transport model were also investigated together with D. Molnar (Purdue University, USA) and M.F. Nagy-Egri (RMI). We constructed parametrizations of nonlinear 2 $\rightarrow$2 transport model results in 0+1D Bjorken geometry, in order to better understand dissipative phase space corrections in kinetic theory and test simplified models/guesses for those commonly used in the literature. It was deemed most immediately suitable for GPGPU calculations because it mainly involves integration in two dimensions only. We studied, how strongly the initial conditions effect the final Tsallis-like distribution and the flow values. These results were presented at the Zimanyi Winter School

An other interesting result of our thermodynamic investigation is related to Schwarzschild black holes. Here we have proved that introducing the volume as a new thermodynamic variable together with a new interpretation of the Bekenstein-Hawking entropy eliminates the negative heat capacity of the original theory. In a countinously accelerating system, similarities with the Unruh temperature were found.

Development for heavy-ion computer simulations. — In collaboration with the University of Berkeley (USA) and IoPP CCNU (Wuhan, China), we finished to develop the HIJING++ heavy-ion Monte Carlo Generator with G. Papp (ELTE), G.Y. Ma (IoPP CCNU), and X.N. Wang (IoPP CCNU, LBNL). The transplantation of the original, 20 years old code from FORTRAN to C++ programming languages was successful. We built a parallel code, providing faster simulations.

The development of the future Monte Carlo generator for the heavy-ion collisions, HIJING++ were reached the stage. The tuning of the nuclear effect for proton-proton (pp) and proton-nucleus (pA) collisions was finished, and we could present first preliminary physics results on pp and pPb collisions in a large and comprehensive study. The predictions were done for the identified hadron production for pPb collisions at 8.16 TeV cm energy in agreement with the experimental data.

Coordination of the ALICE TPC upgrades. — We coordinate the Hungarian contribution to CERN's largest heavy-ion experiment ALICE. This activity is many-folded: In addition to data analysis, our group plays key role in the construction of the world largest, 90 m^3-volume, GEM-based TPC for the ALICE and the DAQ O2 upgrade projects.

Operation and Management of the ALICE GRID Tier-2 Center. — We extended our storage capacity: currently 3 storage servers are working. We updated the capacity up to 750TB, all configured and switched online by mid 2018.

Coordination of the MGGL. — Together with the Gravitational Wigner Research Group of the Theory department, we coordinated and organized the establishment of the Matra Gravitational and Geophysical Laboratory of Wigner RCP. This is situated in the Gyöngyösoroszi mine and performs various preparational underground measurements for future, third generation gravitational wave detectors. In 2018, we published the long term data analysis for 2016-2018 in a joint paper, which was submitted to Classical and Quantum Gravity. These data were presented for the LIGO/Virgo collaborations, to the Hungarian

Academy of Sciences and on various conferences and workshops. In connection to this, we renovated the Janossy pit at the KFKI campus and we started an improved version of the Eötvös experiment.

Education, PR and future. — Connected to our group we had 5 BSc and 7 MSc students. Our young colleagues participated in young researcher's projects and a 4 TDK theses were submitted for the competition: Andras Leitereg (3rd price OTDK, D. Berenyi) and Adam Takacs (G.G. Barnafoldi) awarded the Excellent student Prize of the ELTE TTK 2018), Kovacs Robert got the "Gyorgyi Geza Prize" of the MTA Wigner RCP.

Peter Posfay and Daniel Berenyi passed the Doctoral exams at the Eotvos Univeristy and they preparing their PhD theses for defense. So far we have 6 young PhD fellow in the research group. Senior colleagues are members of the ELTE, BME, PTE doctoral preogrammes. The following group members participated as guest editors: T. S. Biro as editor-in-chief in EPJ A Hadrons and Nuclei, and guest editor of the Wigner Yearbook 2018.

Group members played key role in the following workshop, conference and seminar organizations: "The Future of Many-Core Computing in Science: GPU Day 2018" and "Lectures of Modern Scientific Programming 2018" at the at Wigner RCP of the HAS; "Mechanika a teridőn" space-time summer School;, Zimanyi Winter School 2018 (Budapest, Hungary). T.S. Biro act as the main organizer of the Wigner Colloquium series for our Institute.

Group members participated in PR activities such as the MAFIHE Schools, the "CERN 25 (HAS), the CREDO tutorial workshop and CERN & Wigner Open Days. We receive regularly invitation by High Schools from Hungary and abroad for PR talks. Besides these activities, we established a good media connection: we participated in several appearances of news, in radio programs, outreach films and on television.

Grants

NKFIH[2] K-123815: Intelligent particle physics: the birth of hadrons (T.S. Biró, 2017-2020)

NKFIH K-124366: Geophysical origin noises in gravitational wave detection (consortium leader: P. Ván, 2017-2020)

NKFIH K-120660: Investigation of the Identified Hadron Production in the Heavy-ion Collisions at the High-luminosity LHC by the ALICE Experiment (G.G. Barnaföldi, 2016-2020)

OTKA K-104260: Particles and intense fields (consortium leader: T.S. Biró, 2012-2017)

OTKA K-116197: Heat transport in extreme media and systems, consortium leader, (P. Ván, 2015-2019)

OTKA K-109462: Theoretical investigations of the strongly interacting matter produced at FAIR (CBM, PANDA) and NICA (Dubna) (Gy. Wolf, 2014-2018)

PANDA and NICA (Dubna) (Gy. Wolf, 2014-2018)

[2] NKFIH: National Research, Development and Innovation Office

International cooperation

HIC for FAIR program participation with Frankfurt University, FIAS and GSI Darmstadt (T.S. Biro, Gy. Wolf)

UKRAINIAN – HUNGARIAN MTA-UA bilateral mobility program NKM-81/2016 (Hungarian leader: T.S. Biro, Ukrainian leader: L. Jenkovszky).

CERN ALICE experiment, (G.G. Barnafoldi, group leader, and P. Levai)

CERN ALICE TPC and O2 upgrade project, (G.G. Barnafoldi Wigner group leader, 2015-2018)

THOR EU COST CA15213 action (Hungarian Representatives: G.G. Barnafoldi – Core member, M. Csanad, 2016-2019)

PHAROS EU COST CA16214 action (Hungarian Representatives: G.G. Barnafoldi – WG Task leader, M. Vasuth, 2017-2021)

Long-term visitors

D. Molnar (G.G. Barnafoldi, 5 months), M. Bejger (G.G. Barnafoldi, M. Vasuth 1 month), Y. Mao (G.G. Barnafoldi, 1 week), A. Ortiz Velasquez (G.G. Barnafoldi, 1 week), G. Paic (G.G. Barnafoldi, 1 week), L. Zhu (P. Lévai 1 week), Y. Mao (P. Levai 1 week)

Publications

Articles

1. Albacete JL et al. incl. Barnaföldi GG, Bíró G, Gyulassy M, Harangozó SM, Lévai P [42 authors]: Predictions for cold nuclear matter effects in p+Pb collisions at $\sqrt{s_{NN}}$ =8.16 TeV. ***NUCL PHYS A* 972:** 18-85 (2018)
2. Balassa G, Kovács P, Wolf G: A statistical method to estimate low-energy hadronic cross sections. ***EUR PHYS J A* 54**:2 25/1-13 (2018)
3. Berényi D, Leitereg A, Lehel G: Towards scalable pattern-based optimization for dense linear algebra. ***CONCURR COMP-PRACT E* 3**0:22 e4696/1-14 (2018)
4. Berényi D, Lévai P: Chiral magnetic effect in the Dirac–Heisenberg–Wigner formalism. ***PHYS LETT B* 782**: 162-166 (2018)
5. Biró T, Greiner C, Müller B, Rafelski J, Stöcker H: Topical issue on frontiers in nuclear, heavy ion and strong field physics. ***EUR PHYS J A* 54**:2 31/1-3 (2018)
6. Biró TS, Telcs A, Neda Z: Entropic distance for nonlinear master equation. ***UNIVERSE* 4**:1 10/1-8 (2018)
7. Biró TS, Czinner VG, Iguchi H, Ván P: Black hole horizons can hide positive heat capacity. ***PHYS LETT B* 782**: 228-231 (2018)
8. Biró TS, Schram Z, Jenkovszky L: Entropy production during hadronization of a quark-gluon plasma. ***EUR PHYS J A* 54**:2 17/1-10 (2018)
9. Biró TS, Néda Z: Unidirectional random growth with resetting. ***PHYSICA A* 499**: 335-361 (2018)
10. Divotgey F, Kovács P, Giacosa F, Rischke DH: Low-energy limit of the extended Linear Sigma Model. ***EUR PHYS J A* 54**:1 5/1-14 (2018)
11. Fülöp T, Kovács R, Lovas Á, Rieth Á, Fodor T, Szücs M, Ván P, Gróf Gy: Emergence of non-Fourier hierarchies. ***ENTROPY* 20**:11 832/1-13 (2018)

12. Gora D et al. incl. Kovács P [21 authors]: Cosmic-ray extremely distributed observatory: status and perspectives. ***UNIVERSE* 4**:11 111/1-7 (2018)
13. Kovács R, Ván P: Second sound and ballistic heat conduction: NaF experiments revisited. ***INT J HEAT MASS TRAN* 117**: 682-690 (2018)
14. Kovács R: Analytic solution of Guyer-Krumhansl equation for laser flash experiments. ***INT J HEAT MASS TRAN* 127**: 631-636 (2018)
15. Olbrich L, Zétényi M, Giacosa F, Rischke DH: Influence of the axial anomaly on the decay N(1535) $\rightarrow$ N η. ***PHYS REV D* 97**:1 014007/1-18 (2018)
16. Pósfay P, Barnaföldi GG, Jakovác A: Effect of quantum fluctuations in the high-energy cold nuclear equation of state and in compact star observables. ***PHYS REV C* 97**:2 025803/1-5 (2018)
17. Pósfay P, Barnaföldi GG, Jakovác A: The effect of quantum fluctuations in compact star observables. ***PUBL ASTRON SOC AUST* 35**: e019/1-6 (2018)
18. Révai J: Are the chiral based $\bar{K}N$ potentials really energy-dependent? ***FEW-BODY SYST* 59**:4 49/1-6 (2018)
19. Rieth Á, Kovács R, Fülöp T: Implicit numerical schemes for generalized heat conduction equations. ***INT J HEAT MASS TRAN* 126**: 1177-1182 (2018)
20. Rogolino P, Kovács R, Ván P, Cimmelli VA: Generalized heat-transport equations: parabolic and hyperbolic models. ***CONTINUUM MECH THERM* 30**:6 1245-1258 (2018)
21. Shen K-M, Biró TS, Wang E-K: Different non-extensive models for heavy-ion collisions. ***PHYSICA A* 492:** 2353-2360 (2018)
22. Wolf G, Balassa G, Kovács P, Zétényi M, Lee SH: Mass shift of charmonium states in $\bar{p}A$ collision. ***PHYS LETT* B** 780: 25-28 (2018)
23. Zétényi M, Speranza E, Friman B: Polarization and dilepton angular distribution in pion-nucleon collisions. ***FEW-BODY SYST* 59**:6 UNSP 138/1-7 (2018)
24. Zétényi M, Wolf G: Influence of anisotropic Λ/Σ creation on the Ξ^- multiplicity in subthreshold proton–nucleus collisions. ***PHYS LETT B* 785**: 226-231 (2018)

Conference proceedings

25. Bíró G, Barnaföldi GG, Biró TS, Shen K: Mass hierarchy and energy scaling of the Tsallis - Pareto parameters in hadron productions at RHIC and LHC energies. ***EPJ WEB CONF* 171**: 14008/1-4 p. (2018) (*Proc. 17th International Conference on Strangeness in Quark Matter (SQM 2017), Utrecht, The Netherlands, July 10-15, 2017*.Eds.: Mischke A, Kuijer P)
26. Wolf G, Balassa G, Kovács P, Zétényi M, Lee SH: Charmonium excitation functions in $\bar{p}A$ collisions. ***ACTA PHYS POL B PROC SUPPL* 11**:3 531-536 (2018) (Excited QCD 2018, Kopaonik, Serbia, 11-15 March 2018)
27. Zétényi M, Wolf Gy: Subthreshold Ξ^- production in proton-nucleus collisions in a BUU model. ***EPJ WEB CONF* 171**: 19006/1-4 (2018) (*Proc. 17th International Conference on Strangeness in Quark Matter (SQM 2017), Utrecht, The Netherlands, July 10-15, 2017*.Eds.: Mischke A, Kuijer P)

Book chapter

28. Ván P: Weakly nonlocal non-equilibrium thermodynamics: The Cahn-Hilliard equation. In: *Generalized Models and Non-classical Approaches in Complex Materials 1, Advanced Structured Materials.* Eds.: Altenbach H, Pouget J, Rousseau M, Collet B, Michelitsch T, vol 89, pp 745-760, Springer, Cham

Other

29. Biró T, Greiner C, Müller B, Rafelski J, Stöcker H: Topical issue on frontiers in nuclear, heavy ion and strong field physics. ***EUR PHYS J A* 54**:2 31/1-3 (2018)
30. Ván P, Fülöp T:The 14th Joint European Thermodynamics Conference (JETC 2017) ***J NON-EQUIL THERMODY* 43**:2 87-87 (2018)

See also: R-A.4, R-L.2

ALICE Collaboration

Due to the vast number of publications of the large collaborations in which the research group participated in 2018, here we list only a short selection of appearences in journals with the highest impact factor.

1. Acharya S et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Bíró G, Boldizsár L, Hamar G, Kiss G, Kőfaragó M, Lévai P, Lowe A, Oláh L, Pochybova S, Varga D, Vértesi R [1040 authors]: D-meson azimuthal anisotropy in midcentral Pb-Pb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV. ***PHYS REV LETT* 120**:10 102301/1-13 (2018)
2. Acharya S et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Bíró G, Boldizsár L, Hamar G, Kőfaragó M, Lévai P, Lowe A, Pochybova S, Varga D, Vértesi R [1016 authors]: Dielectron production in proton-proton collisions at $\sqrt{s}$ = 7 TeV. ***J HIGH ENERGY PHYS* 2018**:9 064/1-47 (2018)
3. Acharya S et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Bíró G, Boldizsár L, Hamar G, Kőfaragó M, Lévai P, Lowe A, Pochybova S, Varga D, Vértesi R [1015 authors]: Anisotropic flow of identified particles in Pb-Pb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV. ***J HIGH ENERGY PHYS* 2018**:9 006/1-46 (2018)
4 Acharya S et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Bíró G, Boldizsár L, Hamar G, Kőfaragó M, Lévai P, Lowe A, Pochybova S, Varga D, Vértesi R [1013 authors]: Inclusive J/ψ production at forward and backward rapidity in p-Pb collisions at $\sqrt{s_{NN}}$ = 8.16 TeV. ***J HIGH ENERGY PHYS* 2018**:7 160/1-27 (2018)
5. Acharya S et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Bíró G, Boldizsár L, Hamar G, Kőfaragó M, Lévai P, Lowe A, Pochybova S, Varga D, Vértesi R [1003 authors]: Energy dependence and fluctuations of anisotropic fow in Pb-Pb collisions at $\sqrt{s_{NN}}$ = 5.02 and 2:76 TeV. ***J HIGH ENERGY PHYS* 2018**:7 103/1-39 (2018)
6. Acharya S et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Bíró G, Boldizsár L, Hamar G, Kőfaragó M, Lévai P, Lowe A, Pochybova S, Varga D, Vértesi R [1025 authors]: Λ_c^+production in pp collisions at √s=7 TeV and in p-Pb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV. ***J HIGH ENERGY PHYS* 2018**:4 108/1-48 (2018)
7. Acharya S et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Bíró G, Boldizsár L, Hamar G, Kőfaragó M, Lévai P, Lowe A, Pochybova S, Varga D, Vértesi R [1003 authors]: Measurement of D^0, D^+, D^{*+} and D s^+ production in Pb-Pb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV. ***J HIGH ENERGY PHYS* 2018**:10 174/1-35 (2018)
8. Acharya S et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Bíró G, Boldizsár L, Hamar G, Kiss G, Varga-Kőfaragó M, Lévai P, Lowe A, Oláh L, Pochybova S, Varga D, Vértesi R [1013 authors]: Transverse momentum spectra and nuclear modification factors of charged particles in pp, p-Pb and Pb-Pb collisions at the LHC. ***J HIGH ENERGY PHYS* 2018**:11 13/1-33 (2018)

9. Acharya S et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Bíró G, Boldizsár L, Hamar G, Kőfaragó M, Lévai P, Lowe A, Pochybova S, Varga D, Vértesi R [1016 authors]: Measurements of low-p T electrons from semileptonic heavy-flavour hadron decays at mid-rapidity in pp and Pb-Pb collisions at $\sqrt{s_{NN}}$ = 2.76 TeV. ***J HIGH ENERGY PHYS*** **2018**:10 61/1-30 (2018)
10. Acharya S et al. incl. Barnaföldi GG, Bencédi G, Berényi D, Bíró G, Boldizsár L, Hamar G, Kőfaragó M, Lévai P, Lowe A, Pochybova S, Varga D, Vértesi R [1017 authors]: Medium modification of the shape of small-radius jets in central Pb-Pb collisions at $\sqrt{s_{NN}}$ = 2.76 TeV. ***J HIGH ENERGY PHYS*** **2018**:10 139/1-29 (2018)
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R-E. Holographic quantum field theory

"Momentum" Research Team

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Subtitle. — Field theoretical derivation of Lüscher's formula and calculation of finite volume form factors

Quantum Field Theories play an important role in many branches of physics. On the one hand, they provide the language in which we formulate the fundamental interactions of Nature including the electro-weak and strong interactions. On the other hand, they are frequently used in effective models appearing in particle, solid state or statistical physics. In most of these applications the physical system has a finite size: scattering experiments are performed in a finite accelerator/detector, solid state systems are analyzed in laboratories, even the lattice simulations of gauge theories are performed on finite lattices etc. The understanding of finite size effects is therefore unavoidable and the ultimate goal is to solve QFTs for any finite volume. Fortunately, finite size corrections can be formulated purely in terms of the infinite volume characteristics of the theory, such as the masses and scattering matrices of the constituent particles and the form factors of local operators.

For a system in a box of finite sizes the leading volume corrections are polynomial in the inverse of these sizes and are related to the quantization of the momenta of the particles. In massive theories the subleading corrections are exponentially suppressed and are due to virtual processes in which virtual particles ``travel around the world'.

The typical observables of an infinite volume QFT (with massive excitations) are the mass spectrum, the scattering matrix, the matrix elements of local operators, i.e. the form factors, and the correlation functions of these operators. The mass spectrum and the scattering matrix is the simplest information, which characterize the QFT on the mass-shell. The form factors are half on-shell half off-shell data, while the correlation functions are completely off-shell information. These can be seen from the Lehmann-Symanzik-Zimmermann (LSZ) reduction formula, which connects the scattering matrix and form factors to correlation functions: The scattering matrix is the amputated momentum space correlation function on the mass-shell, while for form factors only the momenta, which correspond to the asymptotic states are put on shell. Clearly, correlation functions are the most general objects as form factors and scattering matrices can be obtained from them by restriction. Alternatively, however, the knowledge of the spectrum and form factors provides a systematic expansion of the correlation functions as well.

The field of two dimensional integrable models is an adequate testing ground for finite size effects. These theories are not only relevant as toy models, but, in many cases, describe highly anisotropic solid state systems and via the AdS/CFT correspondence, solve four dimensional gauge theories. Additionally, they can be solved exactly and the structure of the solution provides valuable insight for higher dimensional theories.

The finite size energy spectrum has been systematically calculated in integrable theories. The leading finite size correction is polynomial in the inverse of the volume and originates from momentum quantization. The finite volume wave-function of a particle has to be periodic, thus when moving the particle around the volume, *L*, it has to pick up the *ipL* translational phase. If the theory were free this phase should be $2\pi n$, in an interacting theory, however, the particle scatters on all the other particles suffering phase shifts, *-ilog(S)*, which adds to the translational phase and corrects the free quantization condition. These equations are called the Bethe-Yang (BY) equations. The energy of a multiparticle state is simply the sum of infinite volume energies but with the quantized momenta depending on the infinite volume scattering matrix.

The exponentially small corrections are related to virtual processes. In the leading process a virtual particle anti-particle pair appears from the vacuum, one of them travels around the world, scatters on the physical particles and annihilates with its pair. Similar process modifies the large volume momentum quantization of the particles. The total energy contains not only the particles' energies, but also the contribution of the sea of virtual particles. The next exponential correction contains two virtual particle pairs and a single pair which wrap twice around the cylinder. For an exact description all of these virtual processes have to be summed up, which is provided by the Thermodynamic Bethe Ansatz (TBA) equations. TBA equations can be derived (only for the ground state) by evaluating the Euclidean torus partition function in the limit, when one of the sizes goes to infinity. If this size is interpreted as Euclidean time, then only the lowest energy state, namely the finite volume ground state contributes. If, however, it is interpreted as a very large volume, then the partition function is dominated by the contribution of finite density states. Since the volume eventually goes to infinity the BY equations are almost exact and can be used to derive (nonlinear) TBA integral equations to determine the density of the particles, which minimize the partition function in the saddle point approximation. By careful analytical continuations this exact TBA integral equation can be extended for excited states.

The similar program to determine the finite volume matrix elements of local operators, i.e. form factors, is still in its infancy. Since there is a sharp difference between diagonal and non-diagonal form factors they have to be analyzed separately. For nondiagonal form factors the polynomial finite size corrections, besides the already explained momentum quantization, involve also the renormalization of states, to conform with the finite volume Kronecker delta normalization. The polynomial corrections for diagonal form factors are much more complicated, as they contain disconnected terms and recently we managed to prove they exact form conjectured earlier. For exponential corrections the situation is the opposite. Exact expressions for the finite volume one-point function can be obtained in terms of the TBA minimizing particle density and the infinite volume form factors by evaluating the one-point function on an Euclidean torus where one of the sizes is sent to infinity. The analytical continuation trick used for the spectrum can be generalized and leads to exact expressions for all finite volume diagonal form factors. For non-diagonal form factors, however, not even the leading exponential correction is known. The aim of our research was to initiate research into this direction.

We developed a novel framework, which provided direct access both to excited states' energy levels and finite volume form factors. The idea was to calculate the Euclidean torus two-point function in the limit, when one of the sizes was sent to infinity. The exact finite volume two-point function then could be used, similarly to the LSZ formula, to extract the information needed: the momentum space two-point function, when continued analytically to imaginary values, had poles exactly at the finite volume energy levels whose residues were the products of finite volume form factors. Of course, the exact determination of the finite-volume two-point function was hopeless in interacting theories, but developing any systematic expansion lead to a systematic expansion of both the energy levels and the form factors. We analyzed two such expansions in our work: in the first, we expanded the two-point function in the volume, which lead to the leading exponential corrections. We performed the calculation for a moving one-particle state. In the second expansion, we calculated the same quantities perturbatively in the coupling in the sinh-Gordon theory. By comparing the two approaches in the overlapping domain we found complete agreement.

As our final result we could manage to extract the leading exponential volume correction both to the energy level and to the simplest non-diagonal form factor. We compared this energy correction to the expansion of the TBA equation and found complete agreement. The correction contains both the effect of the modification of the Bethe-Yang equation by virtual particles and also these particles' direct contribution to the energy. In the case of the simplest non-diagonal form factor a local operator is sandwiched between the vacuum and a moving one-particle state. Our result for the Lüscher correction is valid for any local operator and has two types of contributions. The first comes from the normalization of the state. Since virtual particles change the Bethe-Yang equations, they also change the finite volume norm of the moving one-particle state. The other correction can be interpreted as the contribution of a virtual particle traveling around the world as displayed on Fig. 1.

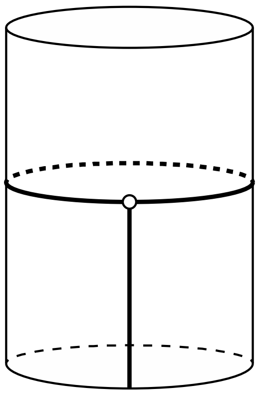

Figure 1. *Graphical interpretation of the Lüscher correction is shown. Solid thick line represents the physical particle which arrives from the infinite past and is absorbed by the operator represented by a solid circle. The trajectory of a virtual (mirror) particle is represented by a half solid, half dashed ellipse. The operator emits this virtual particle, which travels around the world and is absorbed by the operator again leading to a 3-particle form factor.*

Since the appearing 3-particle form factor is infinite, we had to regularize it by subtracting the kinematical singularity contribution. Additionally, however, to this infinite subtraction our calculation revealed an extra finite piece, which was related to the derivative of the scattering matrix. We tested all of our results against second order Lagrangian and Hamiltonian perturbation theory in the sinh-Gordon theory and we obtained perfect agreement. In the future we would like to extend these results for generic non-diagonal finite volume form factor.

Grants

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“Momentum” Program of the HAS (Z. Bajnok 2012-2018)

International cooperations

Gatis+ Reseach Network

Long-term visitor

Haryanto Siahaan, 2017.11.01-2018.06.30

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R-G. “Lendület” innovative gaseous detector development

“Momentum” Research Team

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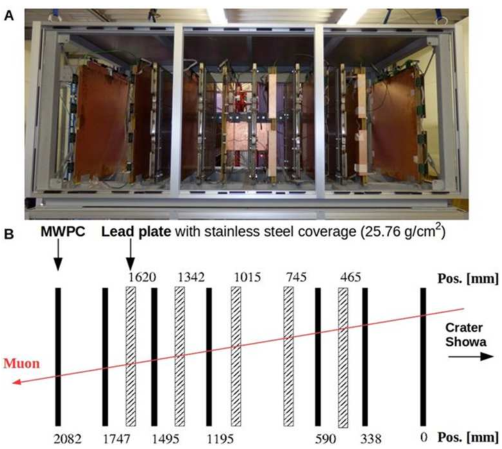
The concluded “Momentum” grant support from the HAS has been converted to a permanent funding starting from this year. The group has concluded commitment to the CERN ALICE TPC Upgrade experiment, as well as completed two deliverables for the H2020 grants BrightnESS and AIDA2020, respectively. An interesting test of General Relativity has been formulated. Using detectors developed by the group, an active volcano imaging has been performed, in collaboration with Tokyo University and the NEC company.

Contributions to CERN ALICE TPC Upgrade Collaboration. — The activities of the group in the TPC Upgrade Collaboration has been concluded, with about 400 large size GEM foils processed in Budapest. The Advanced Quality Assurance testing site which was established, is the second step of the TPC construction after production (at CERN), and the foils were forwarded to Germany and the USA.

Imaging with cosmic muons. — The application of cosmic muons for large-scale imaging has been a research direction in the group in the previous years. An important application for cosmic muons detectors, developed in the last years by the group, is imaging the interior of volcanos. This direction was pursued by Japanese and various European groups. Gaseous tracking detectors, and in our case, a specific type of a Multi-Wire-Proportional-Chamber (MWPC) developed by our group, are highly competitive with the traditional scintillators in terms of cost, weight and power consumption. The detector system has been installed by the Sakurajima volcano in Japan (southern island, see Fig 1), to demonstrate the true applicability and sufficiently low level of background, and to gain experience for the future developments. Presently 4 square meter sensitive area is installed, the largest of its kind in the world, with the results published in Scientific Reports. The japanese NEC company has licensed the



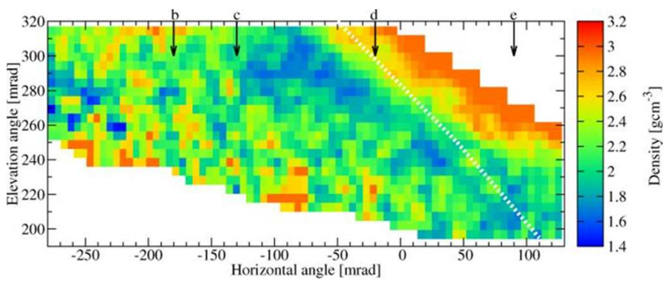


***Figure 1**. Outline of the MOS at Sakurajima, with the image of the Showa crater*

muography observation system (MOS) for research purposes, and continued its licensing rights and funding also this year.

General Relativity effects in storage ring. — A mechanism was proposed in order to perform a General Relativity (GR) experiment using spin-polarized particle beams. The principle of the experiment is the following.

The magnetic moment anomaly, also called g-2, of particles are measured in magnetic storage rings: in a homogeneous magnetic field, the particle spin precesses in the orbital plane at a rate, which is proportional to the magnetic moment anomaly. The electric dipole moment (EDM) of particles are measured in combined magnetic and electric storage rings in which the magnetic spin precession is compensated by a suitably chosen electric field, and such settings are therefore called frozen spin storage rings (Fig.2, left panel). If an EDM of a particle existed, it would torque the spin out of the orbital plane in a frozen spin ring setting. In our paper it was shown that due to General Relativity, Earth's gravitational field also would torque the particle spin out of the orbital plane, similar to an EDM effect (Fig.2, right panel). Therefore, it was proposed to consider the optimization of EDM rings in such a way that the pertinent GR effect can also be detected. This would provide an unusual test of GR in laboratory circumstances: for microscopic particles, at relativistic speeds, along non-geodesic (forced) trajectories, and the tensorial nature of GR would be at test, not merely the gravitational drag.

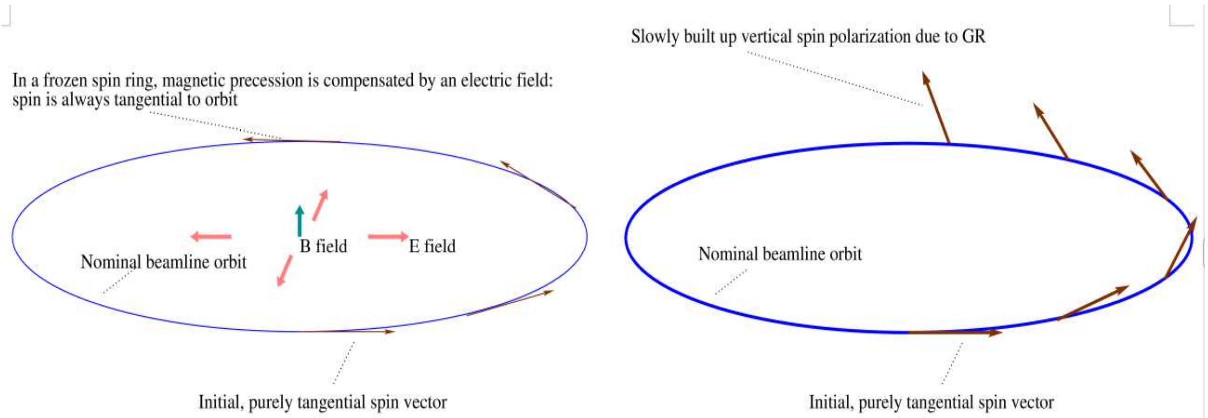


Figure 2. *.Frozen spin muon experiment, and precession effect due to General Relativity effect*

Investigation of neutron scattering. — In order to quantify the neutron scattering in the ESS Multi-Blade detector, highly detailed simulations were performed and compared to measurements, shown in Fig.3. This study has revealed that the scattering (causing background and degradation of image contrast) is extremely small, matching the ESS requirements.

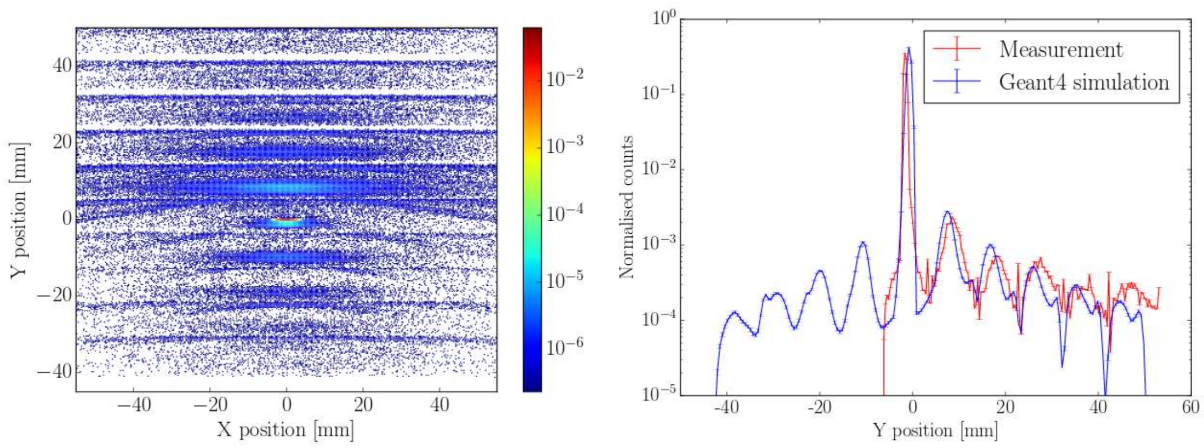


Figure 3. *Scattered neutron position for the Multi Blade detector (in the plane vertical to the beam, left panel), and comparison of the simulations to actual measurement (right panel)*

Grants

ADIA-2020 (Advanced European Insfrastructures for Detectors at Accelerators), H2020 support (D. Varga, 2015-2018)

BrightnESS (Research Infrastructure for ESS), H2020 support (D. Varga, 2015 - 2018)

NKFIH-FK 123959, (A. László, 2017-2020)

Japanese-Hungarian TéT, Serbian-Hungarian TéT, (2017-2019)

International cooperation

CERN NA61 Collaboration (A. László), CERN RD51 Collaboration (D. Varga), CERN ALICE TPC Upgrade Collaboration (D. Varga, G. Hamar, Á. Gera)

Earthquake Research Institute, Tokyo Uni., Muography for Volcano Monitoring (L. Oláh, G. Hamar, Á. Gera, G. Nyitrai, D. Varga)

University of Novi Sad (Serbia), Novel Imaging Methods (G. Hamar, D. Varga)

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See also: R-B ALICE Collaboration (Boldizsár L, Hamar G, Oláh L, Varga D)

R-I. Femtosecond spectroscopy and X-ray spectroscopy

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Developing light-activated functional molecules has been a major goal in molecular engineering, as such systems hold the promise for solutions to many technological problems ranging from IT to sustainable development. Relevant efforts have been focused on engineering complexes of the abundant and environment-friendly iron, particularly on the ubiquitous model systems with polypyridine ligands. The first steps for developing efficient light-activated functional molecules is to obtain a thorough understanding of their potential energy surfaces (PES), and unveil the relaxation pathways on them after the excitation. We report on some theoretical and experimental results on iron based molecules which shall assist to open new paths for developing molecular systems which are rather promising for applications .

Quantum nuclear wavepacket simulations of photoexcited Fe-carbene complexes. — Determining the possible photorelaxation pathways and estimating the lifetimes of the excited states is necessary for revealing the mechanism in functional molecules. A theoretical approach to this requires the simulation of the photorelaxation process, whereas for systems with a high density of excited states, such as several transition metal complexes, it might be necessary to explicitly account for the excitation process as well. Continuing our previous studies of iron complexes suggested as substitutes for the expensive and environmentally unfriendly rare earth-based photosensitizers for light-harvesting systems we report taking this aspect into account in the ultrafast excited state relaxation dynamics of the $[Fe(btbip)_2]^{2+}$ and $[Fe(bmip)_2]^{2+}$ complexes (Fig.1).

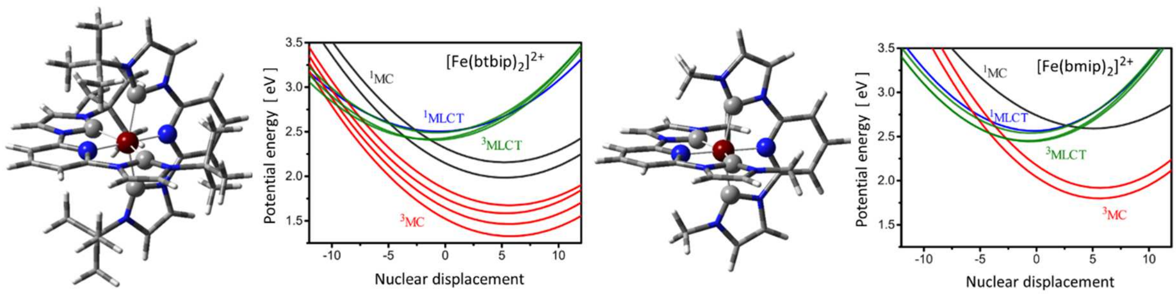

Figure 1. *Molecular structures and potential energy curves for some excited states along the lowest frequency breathing vibrational mode of* $[Fe(btbip)_2]^{2+}$ *(btbip = 2,6-bis(3-tert-butyl-imidazole-1-ylidene)pyridine) (left) and* $[Fe(bmip)_2]^{2+}$ *(bmip = 2,6-bis(3-methyl-imidazole-1-ylidene) pyridine) (right). (N and C atoms are indicated by blue and grey colors, respectively.)*

We performed quantum dynamics simulations in a four dimensional space spanned by the vibrational normal modes most relevant to the transitions. The current, improved description explicitly includes the interaction with the pump laser field in the Hamiltonian of the system in the semiclassical dipole approximation using transition dipole moments (TDM) obtained by the same time-dependent density functional theory (TD-DFT) method (B3LYP*/TZVP) used also for computing the potential energy surfaces and the spin-orbit couplings (SOCs). The simulations were performed with the multi-configurational time-dependent Hartree (MCTDH) method in the vibrational coupling Hamiltonian (VCHAM) formalism. In this formalism the SOCs and TDM vectors are directly determined by TD-DFT, while the non-adiabatic coupling terms and the parameters of the multidimensional potential energy surfaces are determined by fitting to TD-DFT adiabatic potential energy values. In both molecules, the optically bright singlet metal-to-ligand charge transfer state (^{1}MLCT), as well as the energetically closest singlet metal-centred (^{1}MC) states are degenerate, showing E symmetry. We have demonstrated that the spin-vibronic model, constructed directly from electronic structure calculations as described above, can exhibit erroneous, polarization-dependent relaxation dynamics for such degenerate states due to artificial interference of coupled relaxation pathways. We have shown that this problem stems from an incorrect description of the excitation of the ground state nuclear wavepacket into electronically degenerate states. The reason for this deficiency is that the simulation of the excitation process lacks rotational invariance implied by the symmetry of degenerate states. This translates into unphysical behavior through the nonadiabatic couplings among these states. We have demonstrated that a proper complex representation of TDMs is necessary to ensure rotational invariance of the excitation. This eliminates the unphysical interferences and thus produces correctly polarization-independent excited-state dynamics for both investigated complexes. Fig.2 shows the population dynamics for four simulations with different laser polarizations for which - without the correction - we obtained more than 20% deviations in excited state populations at 2 ps after the excitation and a difference of almost a factor of three in relaxation times.

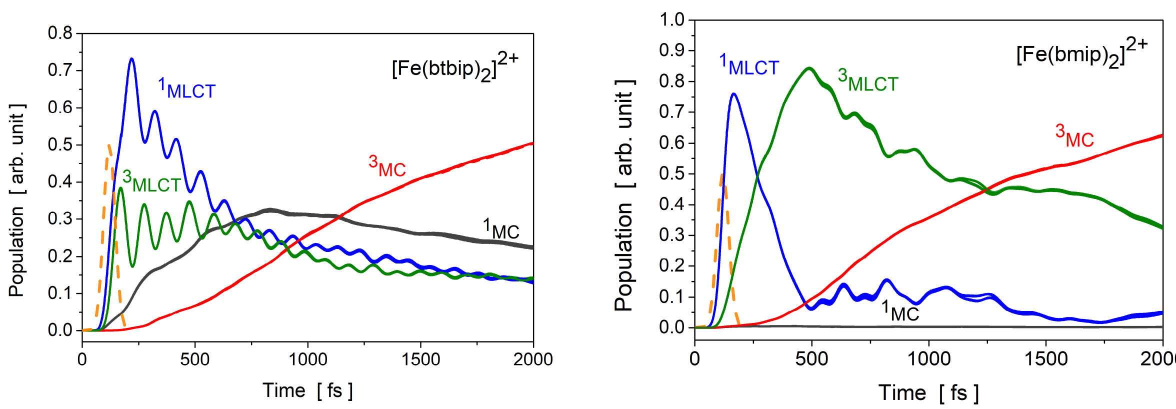

Figure 2. *Results of the simulations: Excited state populations as a function of time for the* $[Fe(btbip)_2]^{2+}$ *(left) and* $[Fe(bmip)_2]^{2+}$ *(right) complexes following excitation by a 485 nm, 60 fs Gaussian pulse with four different laser polarizations. (The temporal intensity profile of the laser pulse is indicated by dashed orange line.) Due to the corrected description of the excitation process, no polarization dependence is observed.*

In agreement with related experiments [Liu et.al. Chem. Comm. 49 (2013) 6412] the simulations reveal that an apparently minor structural difference considerably alters the relaxation dynamics in these functional complexes. In the present case, the *tert*-butyl group stabilizes the ^{1}MC states, enabling the ^{1,3}MLCT → ^{1}MC population transfer in addition to the ^{3}MLCT → ^{3}MC pathway, which in turn leads to much faster relaxation of MLCT states. This explains the different photophysical behavior of these otherwise similar complexes, pointing out a crucial issue for tailoring the function in such complexes.

Controlling the relaxation pathway in photoexcited transition metal complexes via substitution and solvent effects. — An alternative way to alter the photophysical properties of transition metal complexes is to shift the potentials with solvent interactions. This can change the intersections of the potentials of and the couplings between different states, which will accordingly influence the transition trajectories and probabilities. Replacing two bipyridine ligands in the frequently studied $[Fe(bpy)_3]^{2+}$ (bpy = 2,2'-bipyridine) by 4 monodentate CN^- ions introduces two effects that allows us to modify the PES. First, the CN^- substitution makes the ligand field stronger, which shifts the MC (metal centered) states to higher energy; second, interaction with protic solvents affects the strength of the Fe−C bonds, which shifts the energy of the MLCT (metal-to-ligand charge transfer) states. We have investigated these effects on the $[Fe(bpy)(CN)_4]^{2-}$ complex, in collaboration with the groups of Prof. Kelly Gaffney (SLAC) and Prof. M. Nielsen (DTU Lyngby), using a combination of transient optical absorption (TOAS) and X-ray emission spectroscopies. The first effect observed is that due to the increase in the ligand field, the MC states are destabilized, thus the potential energy landscape, as well as the relaxation pattern changes completely. While for $[Fe(bipy)_3]^{2+}$, the relaxation follows a pattern the for the full photocycle ^{1}GS $\rightarrow$ ^{1}MLCT$\rightarrow$^{3}MLCT$\rightarrow$^{3}MC $\rightarrow$^{5}MC$\rightarrow$ ^{1}GS, with very short lived excited singlet and triplet states ($\tau < 100$ fs), and a long lived (600 fs) quintet, the field enhancement of the 4 CN ligands shifts up the quintet to an unreachable energy, and makes the triplets longer lived. However, it depends on the solvent which triplet is stabilized. In water, a solvent with strong Lewis acidity/H-bonding ability, the MLCT excited state of $[Fe(bpy)(CN)_4]^{2-}$ decays still rapidly, in less than 100 femtoseconds, forming a quasi-stable metal-centered excited state with 13 picosecond lifetime, while in weak Lewis acid solvents, such as dimethyl sulfoxide (DMSO) or acetonitrile, the same molecule possesses 19 picosecond ^{3}MLCT excited state lifetime and no discernible contribution from MC states. It was shown that the MC excited state in the former case has triplet (^{3}MC) character, unlike other reported six-coordinate Fe(II)-centered

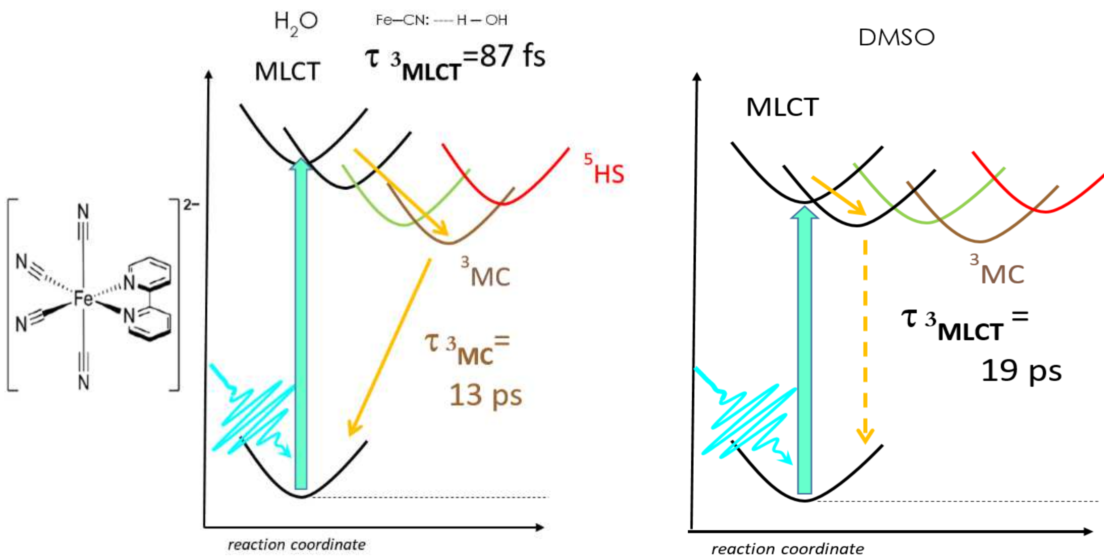

Figure 3. *The $[Fe(bpy)(CN)_4]^{2-}$ molecule (left), and its schematic potential energy curves for water (middle) and DMSO (right) solvents. Yellow arrows show the relaxation pathways. (The full article can be accessed at* http://dx.doi.org/10.1039/c7cp07838b.*)*

coordination compounds with a singlet ground state forming MC quintet (^{5}MC) states. The influence of the solvent on the excited state relaxation dynamics arises from different solvent stabilization of the CN^- ligand, which in turn modifies the relative energies of the MLCT potential energy curves, as shown in Fig. 3. The observed solvent dependent changes in excited state non-radiative relaxation for $[Fe(bpy)(CN)_4]^{2-}$ allows us to infer the influence of the solvent on the electronic structure of the complex.

Following the results detailed above, we have chosen to carry out a similar substitution on another model system, $[Fe(terpy)_2]^{2+}$ (terpy: 2,2':6',2''-terpyridine) complex, whose photophysical behavior is well known. The effect of the terpy – CN ligand substitution should in principle be the similar as described above for the bipyridine analogue, thus it should allow us to verify this type of controlling of the PES, hence the elementary processes of photorelaxation. Our theoretical (TD-)DFT and transient optical absorption studies on the $[Fe(terpy)(CN)_3]^-$ system confirmed relevant variations in the PES and the time evolution, respectively, see the upper part of Fig. 4. Upon the cyanide substitution in $[Fe(terpy)_2]^{2+}$, the calculated triplet and quintet MC states are shifted to higher energies and the solvent effect on the MLCT bands is also reproduced (not shown here). TOAS reflect significantly different behavior compared to the original $[Fe(terpy)_2]^{2+}$, and also some difference from the bipy/CN mixed complex discussed above. Here the ligand field enhancement is somewhat smaller because of the smaller number of CN ligands, thus the quintet MC state is still reached in the relaxation, yet its small yield reflects small branching into this state. During one of the first pilot experiments at the European X-ray Free Electron Laser it was possible to perform a quick feasibility test on aqueous $[Fe(terpy)(CN)_3]^-$ with 515 nm laser excitation and collect a delay scan of difference signals on the Fe Kα lines. The lifetime obtained is fully consistent with that of the major component in the TOAS signal; however, better statistics, longer scan range and the collection of the Kβ spectrum and wide angle scattering are required to fully characterize the excited state dynamics in these molecular systems.

Grants

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2018-1.2.1-NKP-2018-00012: Ultrafast experiments for better functional molecules, nanocircuits and atomic beams (P. Dombi, 2018-2022)

International cooperation

Main cooperations: Prof. C. Bressler, Dr. W. Gawelda (XFEL.EU, Hamburg), Prof. M. M. Nielsen, Dr. K. Haldrup (Copenhagen), Dr. Thomas Penfold (Newcastle), Drs. G. Doumy, A. M. March, S. H. Southworth, L. Young (Argonne), Dr. Jakub Szlatchetko (Kraków), Dr. Chris Milne

(SwissFEL, PSI), Prof. F. M. F. de Groot (Utrecht), Dr. Kelly Gaffney (SLAC), Dr. A. Juhin (Paris) , Dr. T. Katayama (SACLA)

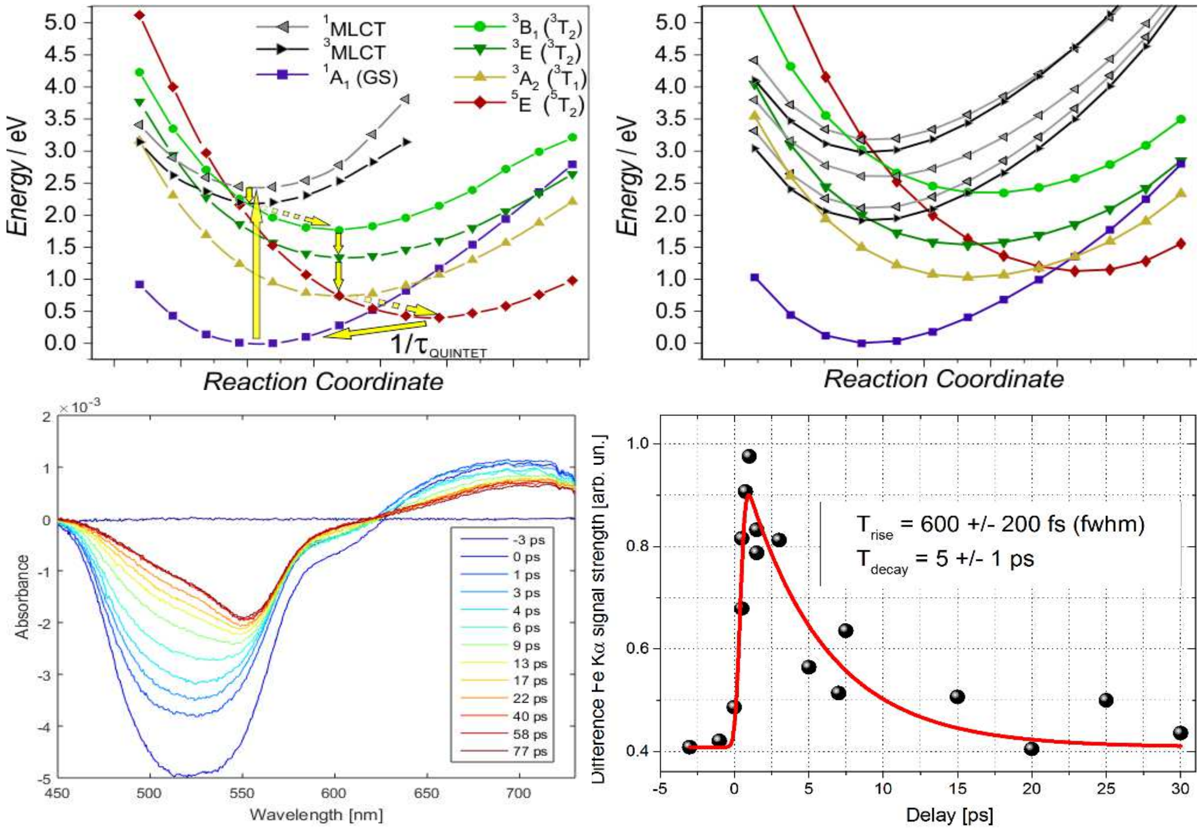

Figure 4. *Top: Calculated PES of the relevant ground-, MLCT, and MC excited states for $[Fe(terpy)_2]^{2+}$ (left) and for $[Fe(terpy)(CN)_3]^-$(right). Bottom: TOAS (left) and pilot XFEL data: Kα XES difference signal of $[Fe(terpy)(CN)_3]^-$ in water as a function of time delay (right).*

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Conference proceeding

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R-J. Functional nanostructures

Wigner Research Group

Dániel Géza Merkel, Gábor Bazsó, László Bottyán[A], István Dézsi[E], Márton Major, Dénes Lajos Nagy[E], Szilárd Sajti

Iron Self-diffusion in Fe_5Ge_3 thin film. — Iron-germanides are widely investigated due to their possible application in nanoelectronics and spintronics applications. The feasibility of these materials in industrial application is highly dependent on their structural stability against temperature, therefore it is indispensable to understand temperature induced diffusion processes in this system. [$^{57}Fe_5Ge_3$(36 Å)/$^{n}Fe_5Ge_3$(62 Å)]$_{10}$ isotope-periodic multilayer has been prepared by molecular beam epitaxy, in order to study iron self-diffusion in Fe_5Ge_3. By using neutron reflectivity technique, which is sensitive to atomic scale diffusion lengths, we have determined the pre-exponent factor and activation energy as D_0 = (8.22 ± 3.8) × 10^{-18} m^2s^{-1} and E_a = (0.28 ± 0.02) eV respectively.

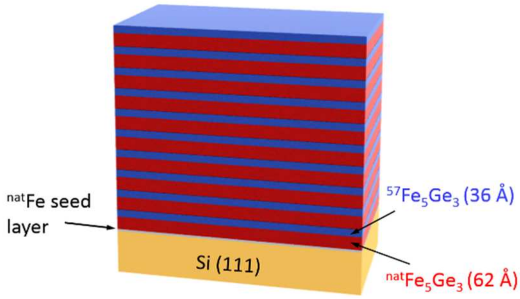

Figure 1. *Layer structure of Fe_5Ge_3 isotope periodic multilayer structure.*

The effect of carboxylic acids on the core/shell structure of iron oxide nanoparticles. — Core/shell nanoparticles have been in the center of scientific interest due to their possible applications in medicine and catalysis. The formation of magnetite/maghemite core/shell structure was studied by Mössbauer-, Raman- and infrared spectroscopies as well as by electronmicroscopy and x-ray diffractometry in coprecipitated iron oxide based nanocomposites functionalized with various carboxylic acids. The core/shell ratio of the nanomagnetites can be changed by the oxidation or the reduction of the particles. It was found that sometimes the phases cannot be determined with Mössbauer spectroscopy at room- or liquid nitrogen temperatures, but only if the samples are measured at the temperature of liquid helium. Our results have shown that alongside with the preparation atmosphere the time of the washing is also crucial parameter during the synthesis of nanomagnetites. We have also found that the previously found correlation between that carboxylic acids and core/shell ratio of the nanomagnetites, can be caused by the different acidity of the carboxylic acids used for the functionalization of the iron oxide nanoparticles. These novel finding can be helpful to adjust the core/shell ratio of the coprecipitated carboxylic acid coated nanomagnetites.

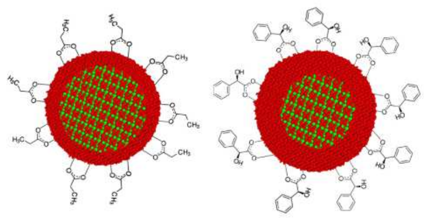

Figure 2*. Schematic illustration of coating with carboxylic acids on nanomagnetite with the change of the thickness of meghemite shell.*

International cooperation

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Long term visitors

- H. Spiering Johannes Gutenberg-Universität Mainz, Institute of Inorganic and Analytical Chemistry, Germany, 16 to 28 October, 2017
- Trân Quôc Dũng, Center for Nuclear Techniques, Vietnam, 26 Dec. 2018 – 08 March 2019

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See also: S-E.1

R-Q. Space physics

Wigner Research Group

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Our research group studies space plasma processes in the Solar System through spacecraft observations and modeling. The main topics of our investigations are Solar System Bodies and Magnetospheres as well as Space Weather. We are involved in numerous space missions at all stages from design to data exploitation in collaboration with the Space Technology research group and our international partners. This year one of these missions reached an important milestone: BepiColombo, a spacecraft to explore Mercury and its environment, was launched on 20th October 2018. Another important achievement of this year is that we helped to create the Europlanet Society, an association to congregate all European planetary scientists and enthusiasts.

Space Weather – Jovian electrons and solar wind structures. — During very low solar activity like in 2007-2008 extremely long-lasting stationary solar wind speed structures can exist near and beyond the Earth for up to 14 solar rotations. These structures modulate the fluxes of both MeV energy Jovian electrons and >50 MeV galactic protons. We attribute this modulation to the formation of a magnetic trap, explaining the 26.1 day period of electron peaks. The effect on electrons and protons is, however, different: while the flux of electrons increases as they are trapped in a magnetic structure, the proton flux decreases due to enhanced convection and adiabatic deceleration during the increase of solar wind speed.

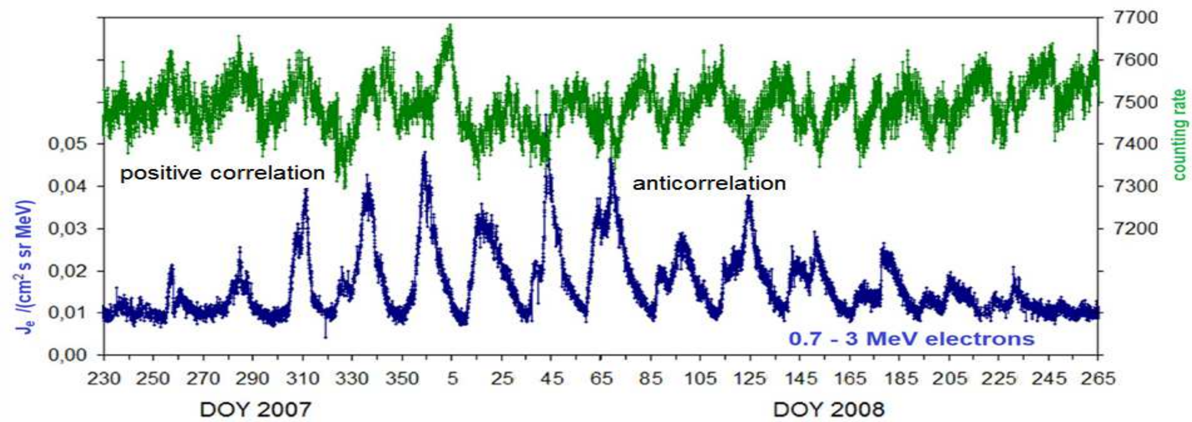

Figure 1.

Space Weather – Space weather propagation. — Participating in the Europlanet 2020-RI project, our group is working on a new solar wind propagation method. Solar wind propagation is a key to predict space weather parameters at certain distances from the Sun. Background solar wind and transients have to be handled separately. For this reason our group has created a database of identified transient events as seen on different space-based instruments and developed a new solar wind propagation method, called Magnetic Lasso propagation.

This is a problem-tailored propagation tool that concentrates on the exact location where the prediction should be most accurate. The method works ballistically, but compared to the simple ballistic approach, the Magnetic Lasso method is based on reconstructing the ideal Parker spiral connecting the target with the Sun by testing a previously defined range of heliographic longitudes. The model takes into account the eventual evolution of stream–stream interactions and handles these with a simple model based on the dynamic pressure difference between the two streams.

The model has the advantage that it can be coded easily and fitted to the problem; it is flexible in selecting and handling input data and requires little running time.

Space Weather – Estimating the solar wind pressure using magnetic field measurements deep inside the magnetosphere. — The solar wind dynamic pressure is an important parameter of space weather, which plays a crucial role in the interaction of the solar wind with the planetary plasma environment. In an induced cometary magnetosphere, the magnetic pressure in the pile-up region (where the magnetic field is compressed and slowed down upstream of the cometary nucleus) is balanced by the external solar wind dynamic pressure.

Our investigations have revealed that the magnetic pressure can be approximated by the magnetic field measurements performed by Rosetta in the inner regions of the induced magnetosphere of comet 67P/Churyumov-Gerasimenko between April 2015 and January 2016. From this, we determined the external solar wind dynamic pressure around the comet. To validate this Rosetta pressure proxy we then compared it to solar wind pressure extrapolated to comet 67P from near-Earth.

Our pressure proxy is useful not only for other Rosetta related studies but also serves as a new, independent input database for space weather propagation to other locations in the Solar System.

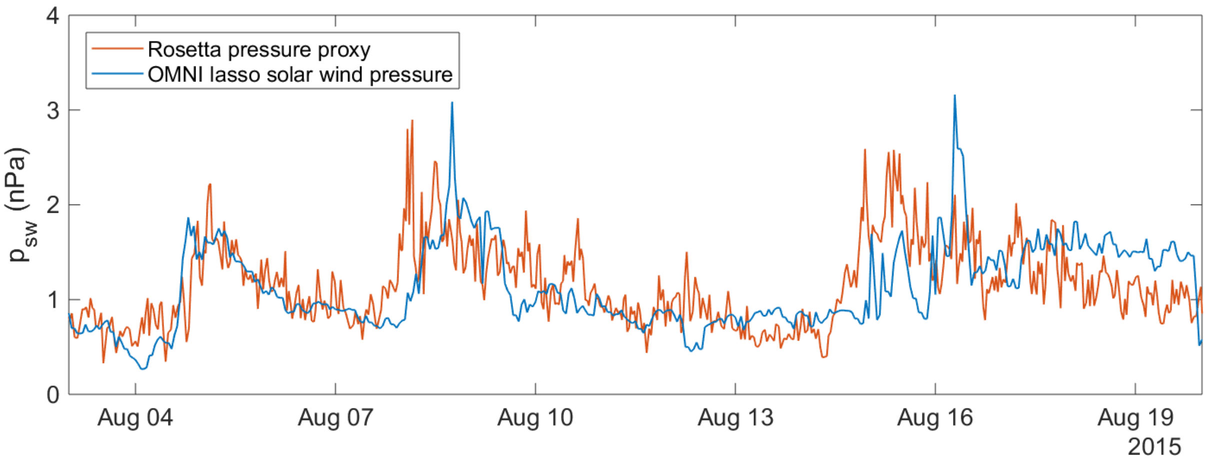

Figure 2.

Magnetospheres – Plasma conditions and the structure of the Jovian ring. — We explored the dynamics of small charged dust particles in Jupiter's innermost magnetosphere and showed that the systematic charge variation of the grains results in surprisingly short lifetimes. Assuming a constant production of small dust particles via continual micrometeoroid bombardment of the larger parent bodies of the main ring, this model reproduces remote sensing observations of the ring/halo region at Jupiter made by Voyager, Galileo, Cassini, and New Horizons spacecraft and observations from the ground by the Keck telescope during ring plane crossings. We use this model to compare the dust impact rates observed by the JUNO mission, which has been traversing the rings multiple times since 2016.

The figure below shows the spatial distribution of the Jovian dust halo for various sized particles, and their flux to the Juno spacecraft following a nearly vertical path (blue lines) crossing the ring plane at 1.06 RJ.

The initial cursory comparison of the data and model prediction seems to match the spatial extent of the Jovian ring/dust halo, at least indicating that our models deciphered the complex dynamics of small charged dust particles near Jupiter.

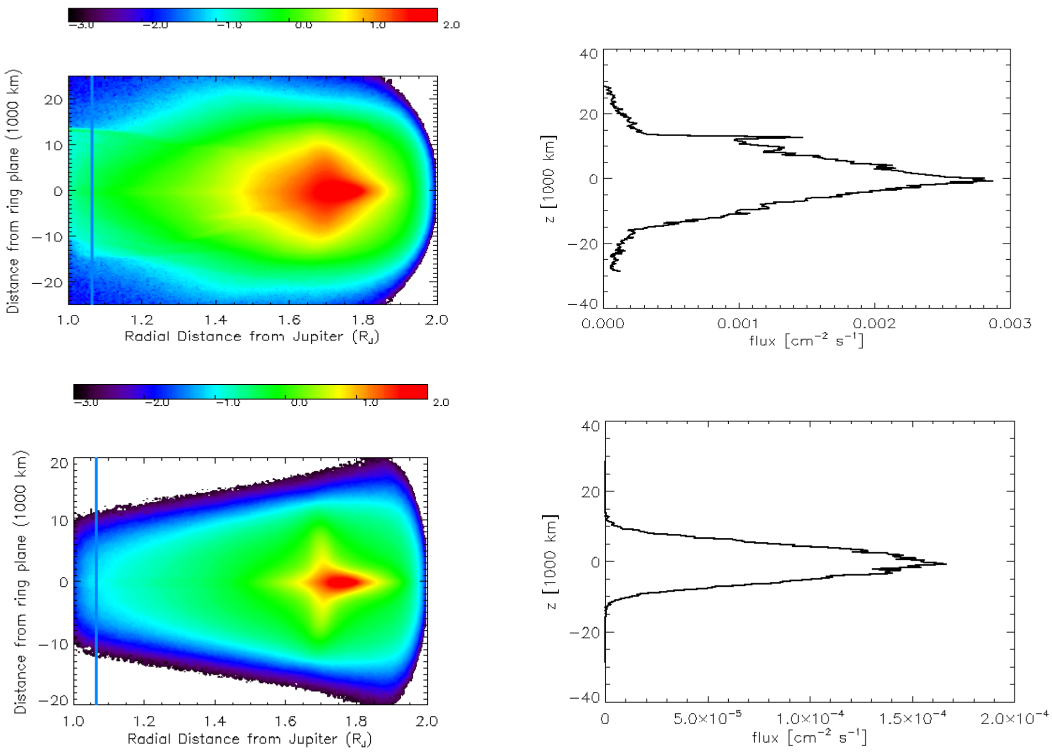

Figure 3.

Magnetospheres – The theory of the diamagnetic cavity of comets. — Recent observations of the Rosetta mission provide comprehensive plasma data about a multitude of diamagnetic cavity crossing events and reveal a surprisingly large diamagnetic cavity around comet Churyumov-Gerasimenko featuring an unforeseen, rich and very dynamic structure. The classical description of the cavity – although very successful in explaining many aspects of the observations – concentrates on solving a single equation in the long distance and zero resistivity limit. We found that exact analytical solutions of the complete set of equations exist for a more general case. These solutions provide new insights into the properties and dynamics of the phenomenon. The generalized solutions show that the magnetic field does not drop to zero immediately inside the cavity, but features a rapid exponential decay instead. Outside the cavity as the distance increases, the magnetic field approaches the classical solution. The plasma velocity first drops rapidly as the plasma enters the cavity boundary; for larger distances, it decreases as 1/r towards its asymptotic value. We can find inward and outward moving solutions possessing distinctly different properties and explaining the dynamic nature of the cavity. The plasma density has a peak just outside the cavity, the density enhancement is more pronounced for weak comets, resulting in stronger than expected interaction and thus larger cavity.

Grants

EU H2020 Europlanet-RI (K. Szegő and A. Opitz, 2015-2019)

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ESA Solar Orbiter Test Data (A. Opitz, G. Erdős 2018-2019)

OTKA FK 128548 Inner Heliosphere (A. Opitz 2018-2022)

János Bolyai Research Scholarship (Z. Németh, 2016-2019)

ÚNKP Bolyai+ Scholarship (Z. Németh, 2018-2019)

International cooperation

International team of the NASA Cassini Plasma Spectrometer (CAPS), (K. Szegő, Z. Németh)

International team of the NASA Cassini Magnetometer (MAG), (G. Erdős)

International team of the NASA STEREO Plasma Spectrometer (PLASTIC), (A. Opitz)

International team of the ESA Rosetta Plasma Consortium (RPC), (K. Szegő, Z. Németh)

International team of the ESA Cluster mission (M. Tátrallyay)

International team of the ESA BepiColombo Particle Detector (SERENA), (K. Szegő)

International team of the ESA Solar Orbiter Magnetometer (MAG), (G. Erdős)

International team of the ESA JUICE Magnetometer (J-MAG), (G. Erdős)

International team of the ESA JUICE Particle Enironment Package (PEP), (K. Szegő)

Europlanet2020-RI, integrating the European planetary science community (K. Szegő, A. Opitz)

University of Colorado, Boulder, USA (A. Juhász)

Lomonosov Moscow State University, Russia (K. Kecskeméty)

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S-A. Strongly correlated systems

"Momentum" Research Team

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In this year, we have continued our research on various strongly correlated systems using the *Density Matrix Renormalization Group* (DMRG), *Matrix Product State* (MPS) and *Tree Tensor Network State* (TTNS) methods. We have also given close to twenty talks on different conferences and seminars, and we have presented some ten posters. In addition, we have further developed our scientific softwares (**Budapest QC-DMRG program package**), which have been used with great success in numerous research institutes and universities around the world for, e.g., simulating material properties of solid-state systems or molecules or for the quantum simulation of the information technology itself. Further algorithmic developments have also been carried out concerning the quantum chemistry DMRG and Coupled-Cluster (CC) algorithms. In addition, in collaboration with Prof. Karol Kowalski, PNNL, Richland, Washington State, USA, we have worked on the migration of the DMRG algorithm into the NWChem (commercial) program package, which ensures the possibility of massive parallelization. In collaboration with guest researchers from the groups of University of Ghent and University of Marburg, we have been working on new algorithmic solutions on the tree-TNS algorithm. As will be presented below, among many others, we have examined strongly correlated electrons in magnetic materials in several quantum phases, exotic quantum phases in ultracold atomic systems, and we have determined multi-orbital correlation and entanglement patterns in molecules, playing important role in chemical compounds.

Numerical and theoretical aspects of the DMRG-TCC method exemplified by the nitrogen dimer. — We have investigated the numerical and theoretical aspects of the coupled-cluster method tailored by matrix-product states. We have investigated chemical properties of the used method, such as energy size extensivity and the equivalence of linked and unlinked formulation. The existing mathematical analysis was elaborated in a quantum chemical framework. In particular, we highlighted the use of a so-called CAS-ext gap describing the basis splitting between the complete active space and the external part. Moreover, the behavior of the energy error as a function of the optimal basis splitting were discussed. We have shown numerical investigations on the robustness with respect to the bond dimensions of the single-orbital entropy and the mutual information, which are quantities that are used to choose the complete active space. Furthermore, we have extended the mathematical analysis with a numerical study on the complete active space dependence of the error.

Ground-state properties of the symmetric single-impurity Anderson model on a ring from Density-Matrix Renormalization Group, Hartree-Fock, and Gutzwiller theory. — We have analyzed the ground-state energy, magnetization, magnetic susceptibility, and Kondo screening cloud of the symmetric single-impurity Anderson model (SIAM) that is characterized by the bandwidth, the impurity interaction strength, and the local hybridization. We have compared Gutzwiller variational and magnetic Hartree-Fock results in the thermodynamic limit with numerically exact data from the DMRG method on large rings.

To improve the DMRG performance, we have used a canonical transformation to map the SIAM onto a chain with half the system size and open boundary conditions. We have compared to Bethe-Ansatz results for the ground-state energy, magnetization, and spin susceptibility that become exact in the wide-band limit. Our detailed comparison have shown that the field-theoretical description is applicable to the SIAM on a ring for a broad parameter range. Hartree-Fock theory gives an excellent ground-state energy and local moment for intermediate and strong interactions. However, it lacks spin fluctuations and thus cannot screen the impurity spin. The Gutzwiller variational energy bound becomes very poor for large interactions because it does not describe properly the charge fluctuations. Nevertheless, the Gutzwiller approach provides a qualitatively correct description of the zero-field susceptibility and the Kondo screening cloud. The DMRG provides excellent data for the ground-state energy and the magnetization for finite external fields. At strong interactions, finite-size effects make it extremely difficult to recover the exponentially large zero-field susceptibility and the mesoscopically large Kondo screening cloud.

Elucidating cation--cation interactions in neptunyl dications using multireference ab initio theory. — Understanding the binding mechanism in neptunyl clusters formed due to cation-cation interactions is of crucial importance in nuclear waste reprocessing and related areas of research. Since experimental manipulations with such species are often rather limited, we have to rely on quantum-chemical predictions of their electronic structures and spectroscopic parameters. We have presented a state-of-the-art quantum chemical study of the T-shaped and diamond-shaped neptunyl(V) and neptunyl(VI) dimers. Specifically, we have scrutinized their molecular structures, solvation effects, the interplay of static and dynamical correlation, and the influence of spin-orbit coupling on the ground state and lowest-lying excited states for different total spin states and total charges of the neptunyl dications. Furthermore, we have used the picture of interacting orbitals (quantum entanglement and correlation analysis) to identify strongly correlated orbitals in the cation-cation complexes that should be included in complete active-space calculations. Most importantly, we have highlighted the complex interplay of correlation effects and relativistic corrections in the description of the ground and lowest-lying excited states of neptunyl dications.

Imaging the Wigner crystal of electrons in one dimension. — The quantum crystal of electrons, predicted more than eighty years ago by Eugene Wigner, is still one of the most elusive states of matter. Recently, it has become possible to design experiments that observe the one-dimensional Wigner crystal directly, by imaging its charge density in real space. The obtained images, of few electrons confined in one-dimension, match those of strongly interacting crystals, with electrons ordered like pearls on a necklace. In order to further support the existence of such a state, we have performed large-scale DMRG calculations on the given sysetm. Comparison to theoretical modeling demonstrates the dominance of Coulomb interactions over kinetic energy and the weakness of exchange interactions. Our experiments together with numerical simulations provide direct evidence for this long-sought electronic state, and open the way for studying other fragile interacting states by imaging their many-body density in real-space.

Analysis of the coupled-cluster method tailored by tensor-network states in quantum chemistry. — We have analyzed the tailored coupled-cluster (TCC) method, which is a multi-reference formalism that combines the single-reference coupled-cluster (CC) approach with a full configuration interaction (FCI) solution covering the static correlation. This covers in particular the high-efficiency coupled-cluster method tailored by tensor-network states (TNS-TCC). For statically correlated systems, we have introduced the conceptually new CAS-ext-gap assumption for multi-reference problems, which replaces the unreasonable HOMO-LUMO gap. We have characterized the TCC function and have shown local strong monotonicity and Lipschitz continuity such that Zarantonello's Theorem yields locally unique solutions fulfilling a quasi-optimal error bound for the TCC method. We have performed an energy error analysis revealing the mathematical complexity of the TCC-method. Due to the basis-splitting nature of the TCC formalism, the error decomposes into several parts. Using the Aubin-Nitsche-duality method, we have derived a quadratic (Newton type) error bound valid for the linear-tensor-network TCC scheme DMRG-TCC and other TNS-TCC methods.

Three-legged tree tensor network states. — We have presented a new variational tree tensor network state (TTNS) ansatz, the three-legged tree tensor network state (T3NS). Physical tensors have been interspersed with branching tensors. Physical tensors have one physical index and at most two virtual indices, as in the matrix product state (MPS) ansatz of the DMRG ansatz. Branching tensors have no physical index, but up to three virtual indices. In this way, advantages of DMRG, in particular a low computational cost and a simple implementation of symmetries have been combined with advantages of TTNS, namely incorporating more entanglement. Our code has been capable of simulating quantum chemical Hamiltonians, and we have presented several proof-of-principle calculations on LiF, N_2, and the bis(μ-oxo) and μ–η^2:η^2 peroxo isomers of $[Cu_2O2]^{2+}$.

Full-configuration interaction quantum Monte Carlo benchmark and multireference coupled-cluster studies for tetramethyleneethane. — We have performed a full-configuration interaction (FCI) quality benchmark calculation for the tetramethyleneethane molecule in the cc-pVTZ basis set employing a subset of complete active-space second-order perturbation theory, CASPT2(6,6), natural orbitals for the FCI quantum Monte Carlo calculation. The results have been in excellent agreement with the previous large-scale diffusion Monte Carlo calculations by Pozun et al. and available experimental results. Our computations have verified that there is a maximum on the potential energy surface (PES) of the ground singlet state (^{1}A) 45° torsional angle, and the corresponding vertical singlet–triplet energy gap is 0.01 eV. We have employed this benchmark for the assessment of the accuracy of Mukherjee's coupled clusters with up to triple excitations (MkCCSDT) and CCSD tailored by the DMRG method. Multireference MkCCSDT with CAS(2,2) model space, though giving good values for the singlet–triplet energy gap, has not been able to properly describe the shape of the multireference singlet PES. Similarly, DMRG(24,25) has not been able to correctly capture the shape of the singlet surface, due to the missing dynamic correlation. On the other hand, the DMRG-tailored CCSD method has described the shape of the ground singlet state with excellent accuracy but for the correct ordering the computation of the zero-spin-projection component of the triplet state ($^3B_1$) is required.

Analysis of electron-correlation effects in strongly correlated systems (N_2 and N_2^+) by applying the DMRG method and quantum information theory. — The dissociation of N_2 and N_2^+ has been studied by using the ab initio density-matrix renormalization-group (DMRG) method. Accurate potential energy surfaces (PESs) have been obtained for the electronic ground states of N_2 ($X_1\Sigma_g^+$) and N_2^+ ($X_2\Sigma_g^+$) as well as for the N_2^+ excited state $B_2\Sigma_u^+$. Inherent to the DMRG approach, the eigenvalues of the reduced density matrix and their correlation functions have been at hand. Thus, we could apply quantum information theory directly and we have investigated how the wave function changes along the PES and depicted differences between the different states. Moreover, by characterizing quantum entanglement between different pairs of orbitals and analyzing the reduced density matrix, we have achieved a better understanding of the multireference character featured by these systems.

Towards a multiconfigurational method of increments. — The method of increments (MoI) allows one to successfully calculate cohesive energies of bulk materials with high accuracy, but it encounters difficulties when calculating dissociation curves. The reason is that its standard formalism is based on a single Hartree–Fock (HF) configuration whose orbitals are localized and used for the many-body expansion. In situations where HF does not allow a size-consistent description of the dissociation, the MoI cannot be guaranteed to yield proper results either. We have addressed the problem by employing a size-consistent multiconfigurational reference for the MoI formalism. This has led to a matrix equation where a coupling derived by the reference itself is employed. In principle, such an approach allows one to evaluate approximate values for the ground as well as excited states energies. While the latter are accurate close to the avoided crossing only, the ground state results are very promising for the whole dissociation curve, as has been shown by the comparison with DMRG benchmarks. We have tested this two-state constant-coupling MoI on beryllium rings of different sizes and studied the error introduced by the constant coupling.

The classification of multipartite quantum correlation. — In multipartite entanglement theory, the partial separability properties have an elegant, yet complicated structure, which becomes simpler in the case when multipartite correlations are considered. We have elaborated this, by giving necessary and sufficient conditions for the existence and uniqueness of the class of a given class-label, by the use of which we have worked out the structure of the classification for some important particular cases, namely, for the finest classification, for the classification based on k-partitionability and k-producibility, and for the classification based on the atoms of the correlation properties.

An entropy production based method for determining the position diffusion's coefficient of a quantum Brownian motion. — Quantum Brownian motion of a harmonic oscillator in the Markovian approximation has been described by the respective Caldeira–Leggett master equation. This master equation can be brought into Lindblad form by adding a position diffusion term to it. The coefficient of this term is either customarily taken to be the lower bound dictated by the Dekker inequality or determined by more detailed derivations on the linearly damped quantum harmonic oscillator. We have explored the theoretical possibilities of determining the position diffusion term's coefficient by analyzing the entropy production of the master equation.

An isolated molecule of iron(II) phthalocyanin exhibits quintet ground-state: a nexus between theory and experiment. — Iron(II) phthalocyanine (FePc) is an important member of the phthalocyanines family with potential applications in the fields of electrocatalysis, magnetic switching, electrochemical sensing, and phototheranostics. Despite the importance of the electronic properties of FePc in these applications, a reliable determination of its ground-state is still challenging. We have presented combined state of the art computational methods and experimental approaches, that is, Mössbauer spectroscopy and Superconducting Quantum Interference Device magnetic measurements to identify the ground state of FePc. While the nature of the ground state obtained with density functional theory depends on the functional, giving mostly the triplet state, multi-reference complete active space second-order perturbation theory and DMRG methods assign quintet as the FePc ground-state in gas-phase. This has been confirmed by the hyperfine parameters obtained from ^{57}Fe Mössbauer spectroscopy performed in frozen monochlorobenzene. The use of monochlorobenzene guarantees an isolated nature of the FePc as indicated by a zero Weiss temperature. The results open doors for exploring the ground state of other metal porphyrin molecules and their controlled spin transitions via external stimuli.

Interaction quench and thermalization in a one-dimensional topological Kondo insulator – We have studied the nonequilibrium dynamics of a one-dimensional topological Kondo insulator, modelled by a p-wave Anderson lattice model, following a quantum quench of the on-site interaction strength. Our goal was to examine how the quench influences the topological properties of the system, therefore our main focus was the time evolution of the string order parameter, entanglement spectrum and the topologically-protected edge states. We have pointed out that postquench local observables can be well captured by a thermal ensemble up to a certain interaction strength. Our results have demonstrated that the topological properties after the interaction quench are preserved at finite times; however, the absolute value of the string order parameter decays in time. These predictions could be directly tested in state-of-the-art cold-atom experiments.

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S-B. Complex systems

Wigner Research Group

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The research activity of Complex Systems research group in 2018 covered various topics in the field of cooperative behavior, phase transitions and nonequilibrium dynamics of systems with many degrees of freedom.

Strong-disorder RG approach — short review of recent developments. — The strong-disorder RG approach for random systems has been extended in many new directions since our previous review of 2005. This year, we have written a colloquium paper to give an overview of these various recent developments. In the field of quantum disordered models, recent progress concerning finite-disorder fixed points for short-ranged models in higher dimensions d > 1, strong-disorder fixed points for long-ranged models, scaling of the entanglement entropy in critical ground states and after quantum quenches, the RSRG-X procedure to construct the whole set of excited states and the RSRG-t procedure for the unitary dynamics in many-body-localized phases, the Floquet dynamics of periodically driven chains, the dissipative effects induced by the coupling to external baths, and Anderson localization models. In the field of classical disordered models, new applications include the contact process for epidemic spreading, the strong-disorder renormalization procedure for general master equations, the localization properties of random, elastic networks, and the synchronization of interacting non-linear dissipative oscillators. Application of the method for aperiodic (or deterministic) disorder is also reviewed.

Transverse-spin correlations of the random transverse-field Ising model. — The random transverse-field Ising model is the prototype of random quantum magnets, which is defined by the Hamiltonian:

$$\mathcal{H} = -\frac{1}{2}\sum_{\langle ij\rangle} J_{ij}\sigma_i^x\sigma_j^x - \frac{1}{2}\sum_i h_i\sigma_i^z \ ,$$

where $\sigma_i^{x,z}$ are Pauli-matrices, i, j denote sites of the lattice and ⟨ij⟩ refers to nearest neighbors. The couplings J_{ij} and transverse fields h_i are independent random numbers. The critical behavior of the model in finite dimensional lattices is governed by infinite-disorder fixed points, several properties of which have already been calculated by the use of the strong-disorder renormalization group (SDRG) method. Here, we have extended these studies and calculated the connected transverse-spin correlation function:

$$G_t(r) = \overline{\langle\sigma_i^z\sigma_{i+r}^z\rangle} - \overline{\langle\sigma_i^z\rangle}\,\overline{\langle\sigma_{i+r}^z\rangle}$$

where the overbar denotes an average over quenched disorder. We have used free-fermionic techniques in d = 1 and a numerical implementation of the SDRG method in d = 1, 2, and 3 dimensions. At the critical point, an algebraic decay of the form $\sim 1/r^{\eta}$ is found, with a decay exponent being approximately $\eta \approx 2+2d$.

Quantum XX model with competing short- and long-range interactions. — We considered the quantum XX model with competing short- and global-range interactions in a one-dimensional lattice, defined by the Hamiltonian:

$$\hat{H} = -J \sum_{j=1}^{L} \left(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y \right) - h \sum_{j=1}^{L} \sigma_j^z - \varepsilon \frac{1}{L} \left(\sum_{j,odd} \sigma_j^z - \sum_{j,even} \sigma_j^z \right)^2 .$$

The nearest-neighbor coupling constant and the strength of the transverse field are denoted by J and h, respectively, and the last term of the r.h.s. represents a global-range antiferromagnetic interaction of strength ε. It is expressed as the square of the staggered magnetization operator:

$$\hat{x} = \frac{1}{L} \left(\sum_{j,odd} \sigma_j^z - \sum_{j,even} \sigma_j^z \right) .$$

This model is equivalent to a Bose-Hubbard model with cavity-mediated global-range interactions in the hard-core-boson limit, which has experimental relevance in terms of cold atoms in an optical lattice in the presence of a high-finesse optical resonator, an optical cavity. Using fermionic techniques, the problem was solved exactly in one dimension in the thermodynamic limit. The ground-state phase diagram consists of two ordered phases: ferromagnetic (F) and antiferromagnetic (AF), as well as an XY phase having quasi-long-range order, see Fig. 1. We have also studied quantum relaxation after sudden quenches. Quenching from the AF phase to the XY region, remanent AF order is observed below a dynamical transition line. In the opposite quench, from the XY region to the AF phase beyond a static

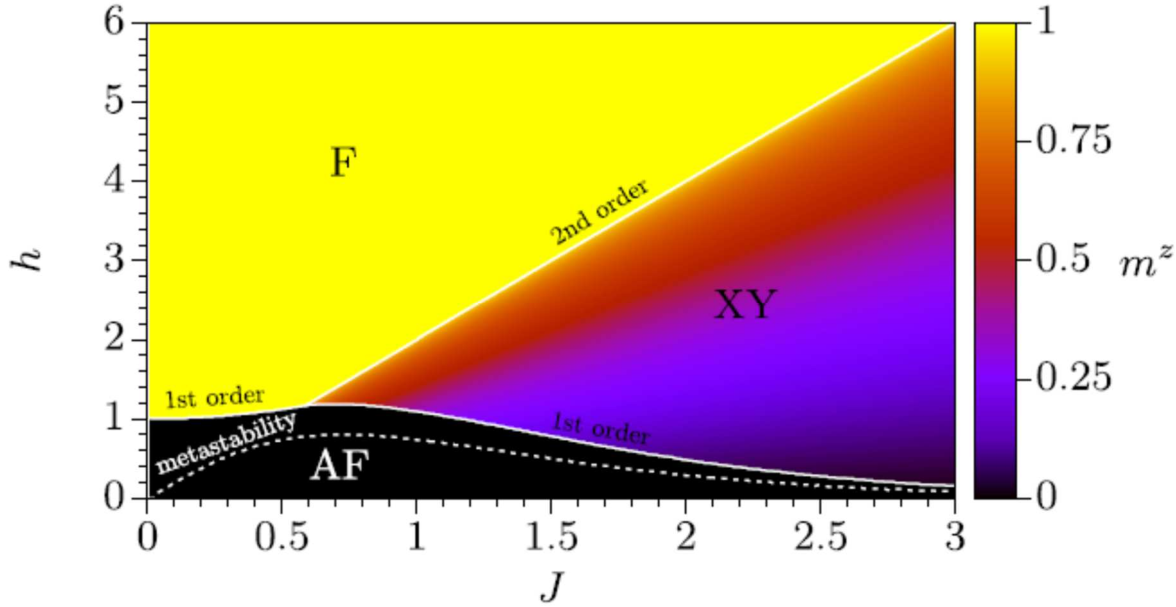

Figure 1. Phase diagram of the quantum XX model with cavity-induced global-range interactions of strength ε = 1. The color codes indicate the value of the staggered magnetization, x, and that of the longitudinal magnetization, m^z.

metastability line, AF order arises on top of a remanent XY quasi-long-range order, which corresponds to a dynamically generated supersolid state in the equivalent Bose-Hubbard model with hard-core bosons.

Entanglement entropy of disordered quantum wire junctions. — The entanglement properties of extended quantum systems have attracted much interest in the recent decade. One reason for this is that various entanglement measures turned out be sensitive to whether the underlying model is critical or not, moreover, some of these showed universal scaling in critical points. For a subsystem A of a closed system in a pure state, the natural entanglement measure is the entanglement entropy, which is the von Neumann entropy of the reduced density matrix corresponding to the subsystem. An important question is how the inhomogeneities, which break translational invariance, and which are present almost inevitably in real systems, affect the entanglement properties. As a contribution to this field, we considered different disordered lattice models composed of *M* linear chains glued together in a star-like manner, and studied the scaling of the entanglement between one arm and the rest of the system using a numerical strong-disorder renormalization group (SDRG) method. We pointed out that the random XX model and the free-fermion (FF) model with random nearest-neighbor hopping obey different SDRG rules at a junction as opposed to a linear geometry, which is illustrated in Fig. 2. For all studied models, the random transverse-field Ising model (RTIM), the XX spin model, and the FF model, the average entanglement entropy is found to increase with the length *L* of the arms according to the form $S(L)=c_{eff}/6\ln L + \text{const}$. For the RTIM and the XX model, the effective central charge c_{eff} is universal with respect to the details of junction, and only depends on the number *M* of arms. Interestingly, for the RTIM, c_{eff} decreases with *M*, whereas for the XX model it increases. For the latter model, the numerical estimates fit accurately to a form linear in 1/M: $c_{eff}(M)=2\ln 2(1-1/M)$. For the free-fermion model, c_{eff} depends also on the details of the junction, which is related to the sublattice symmetry of the model. In this case, both increasing and decreasing tendency with *M* can be realized with appropriate junction geometries. We have also established upper bounds on the average entanglement entropy of a chain of length L for all the three models under study, which hold universally, irrespective of the other subsystem to which the chain is coupled.

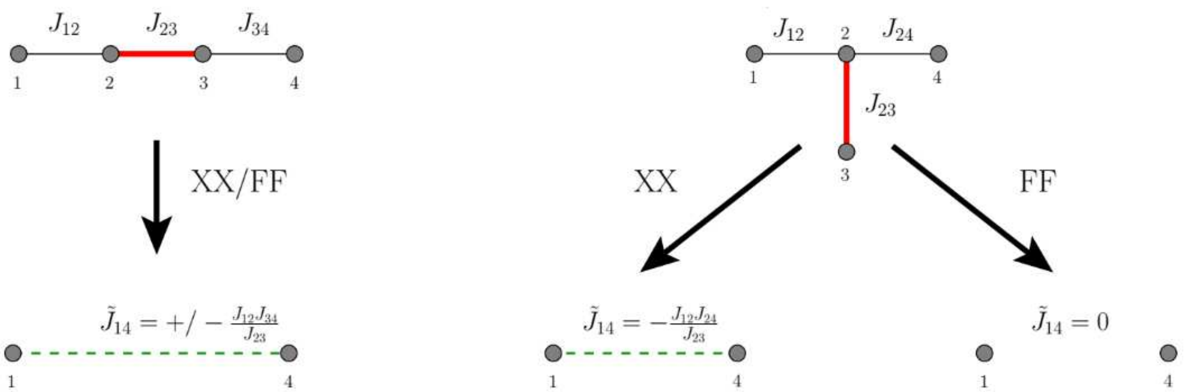

Figure 2. *SDRG steps for the XX model (XX) and free fermions (FF) in the case of two elementary geometries. The sites coupled by the strongest bond (shown in red) are eliminated, while the remaining sites are connected by a weak, effective coupling obtained perturbatively. For the linear configuration the steps for the XX and FF models essentially agree with each other, while for the T shaped geometry they differ.*

Network-based prediction of protein interactions. — As biological function emerges through interactions between a cell's molecular constituents, understanding cellular mechanisms requires us to catalogue all physical interactions between proteins. Despite spectacular advances in high-throughput mapping, the number of missing human protein-protein interactions (PPIs) continues to exceed the experimentally documented interactions. Computational tools that exploit structural, sequence or network topology information are increasingly used to fill in the gap, using the patterns of the already known interactome to predict undetected, yet biologically relevant interactions. Such network-based link prediction tools rely on the Triadic Closure Principle (TCP), stating that two proteins likely interact if they share multiple interaction partners. TCP is rooted in social network analysis, namely the observation that the more common friends two individuals have, the more likely that they know each other. We offered direct empirical evidence across multiple datasets and organisms that, despite its dominant use in biological link prediction, TCP is not valid for most protein pairs. We showed that this failure is fundamental - TCP violates both structural constraints and evolutionary processes. This understanding allowed us to propose a link-prediction principle, consistent with both structural and evolutionary arguments, that predicts yet uncovered protein interactions based on paths of length three (L3). A systematic computational cross-validation showed that the L3 principle significantly outperformed existing link-prediction methods. To experimentally test the L3 predictions, we performed both large-scale high-throughput and pairwise tests, finding that the predicted links test positively at the same rate as previously known interactions, suggesting that most (if not all) predicted interactions are real. Combining L3 predictions with experimental tests provided new interaction partners of FAM161A, a protein linked to retinitis pigmentosa, offering novel insights into the molecular mechanisms that lead to the disease. Because L3 is rooted in a fundamental biological principle, we expect it to have a broad applicability, enabling us to better understand the emergence of biological function under both healthy and pathological conditions.

Collective nonlinear Thomson back-scattering for generating phase-controlled isolated attosecond pulses in the *nm* wavelength range. — We have studied the collectively emitted radiation of a relativistic electron bunch of 10^6 – 10^8 electrons colliding with an intense femtosecond (few-cycle) near-infrared laser pulse. By analytically solving the equation of motion of the electrons interacting with the incoming laser field of arbitrarily high intensity, the exact radiation field stemming from Thomson back-scattering has been calculated in the head-on collision geometry. On the basis of our results, the collective spectrum (containing very high-order harmonics) and the corresponding temporal shape of the radiation emitted by a mono-energetic electron bunch has been determined. It has turned out that for certain, realistic input parameters, single-cycle isolated pulses of ca. 20 attoseconds duration can be generated in the XUV – soft x-ray spectral range, including the 2.33–4.37 nm water window. We have also shown that the generated collective radiation is almost linearly polarized, and it is extremely well collimated around the initial velocity of the electron bunch. Moreover, this radiation has a considerable intensity and its carrier envelope phase difference (CEP) is locked to that of the incoming femtosecond laser pulse. The results of the present study allow us to propose a novel source of isolated attosecond XUV – soft x-ray pulses with a well-controlled CEP. Such sources of radiation may be of importance because isolated attosecond XUV pulses make possible to investigate the real-time electron dynamics in atoms, molecules and solids experimentally. Besides, the CEP of the incoming femtosecond laser pulse affects various processes in atomic or molecular systems on this time scale, as has been observed in most of the pioneering experiments. The proposed novel source of isolated attosecond pulses may have several scientific applications, e.g. in performing pump–probe experiments on the attosecond time scale. Fig. 3 illustrates the CEP phase locking which manifests itself in the temporal evolution of the isolated attosecond pulses generated by the Thomson back-scattering of the incoming single-cycle laser pulses with different CEP values.

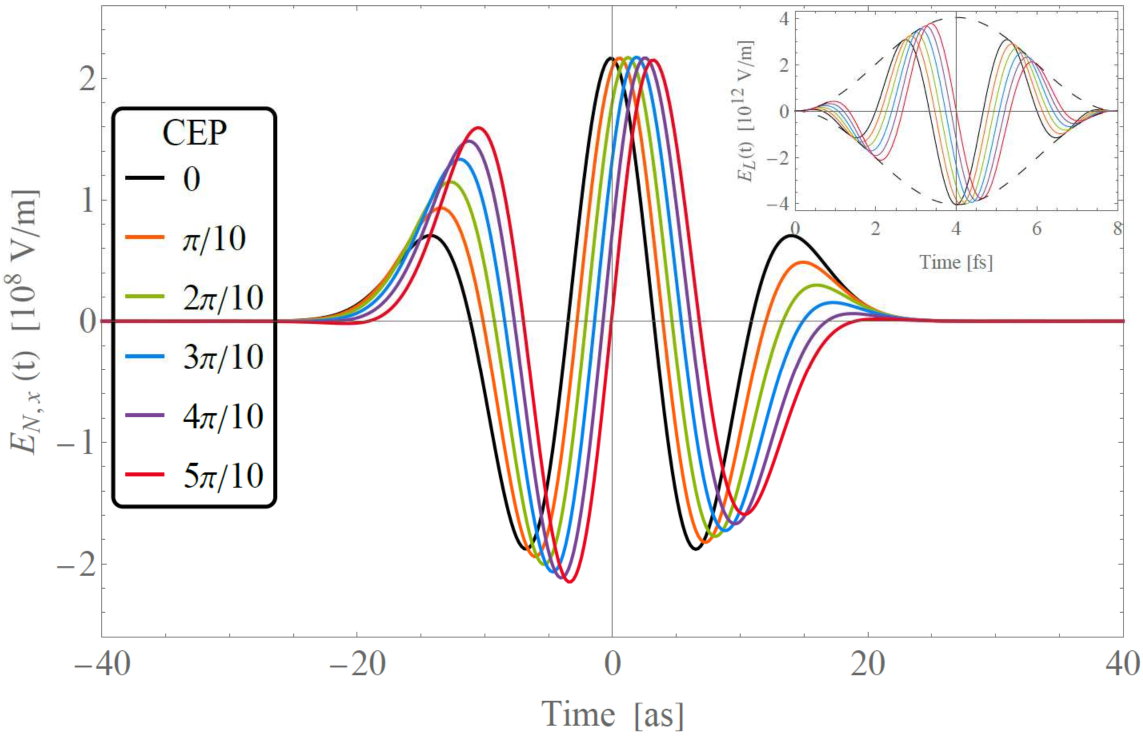

***Figure 3**. Temporal pulse shapes of the isolated attosecond pulses (at distance R_0=2 m from the interaction region), stemming from nonlinear Thomson back-scattering along the polar angle of 180°, for different values of the carrier-envelope phase difference (CEP) of the near-infrared (NIR) laser pulse given in the legend. The inset shows the incoming NIR pulse shapes of different CEP with the corresponding colors. We have considered an 8nm electron bunch of 10^8 electrons, whose initial relativistic factor has been assumed to be γ_0=10. The assumed parameters of the counter-propagating, almost single-cycle laser pulse are λ_L=800 nm, E_0=4×10^{12} V/m.This figure shows that the CEP of the attosecond pulse perfectly follows the CEP of the NIR laser pulse with a phase difference of π. This very simple relationship makes the CEP of these attosecond pulses easily controllable through the CEP of the NIR laser pulse, which is expected to have an importance in attosecond pump-probe experiments.*

Grants

OTKA K-109577: Ordering and dynamics in many-body systems (F. Iglói, 2014-2017)

K_18 (NKFIH) K128989: Many-body systems in and out of equilibrium (R. Juhász, 2018-2022)

International cooperation

Saarland University (Saarbrücken, Germany), Nonequilibrium quench dynamics of quantum systems (F. Iglói, G. Roósz)

National Chengchi University (Taipei, Taiwan), Critical quench dynamics of random spin chains (F. Iglói, G. Roósz)

Northeastern University (Boston, USA), Network-based prediction of protein interactions (I. Kovács)

Kuwait University (Safat, Kuwait), Phase diagram of random, antiferromagnetic spin chains (F. Iglói)

Institut Néel (Grenoble, France) Critical behavior of systems with long-range interactions (F. Iglói)

Université Saclay, CEA, CNRS (Saclay, France) Dynamics of random quantum systems (F. Iglói)

TU München (München, Germany), Entanglement entropy of disordered quantum wire junctions (R. Juhász)

Universität Ulm, Institut für Quantenphysik, Institut für Quantenoptik (Ulm, Germany), Wigner function description of tunneling, focussing waves in quantum mechanics, nano-emitters and single-photon switches (S. Varró)

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Articles

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2. Iglói F, Monthus C: Strong disorder RG approach - a short review of recent developments. ***EUR PHYS J B*** **91**:11 290/1-25 (2018)

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7. Hack S, Varró S, Czirják A: Carrier-envelope phase controlled isolated attosecond pulses in the nm wavelength range, based on coherent nonlinear Thomson-backscattering. ***NEW J PHYS*** **20**: 073043/1-10 (2018)

See also: R-N.2

S-D. Semiconductor nanostructures

"Momentum" Research Team

Ádám Gali, Dávid Beke, Zoltán Bodrog, Émilie Bruyer, András Csóré#, Viktor Ivády, Gyula Károlyházy#, Nain Mukesh#, Bálint Somogyi, Gergő Thiering#, Péter Udvarhelyi#

Design and fabrication of semiconductor nanostructures for bioimaging, quantum computing and 3rd generation photovoltaics. — The research team is active in three main different fields: developing new type of i) biomarkers, ii) quantum bits for quantum information processing, and iii) 3rd generation solar cells. Dániel Áron Major, Dániel Unyi, Balázs Juhász, Titanilla Szilvia Papp, Mátyás Mihály Rudolf and Sebestyén Szabó (BSc and MSc students in chemical engineering and physics) are also active members of the group. Five labor assistants (István Balogh, Péter Rózsa, Dávid Veres, Fanni Oláh, Dóra Zalka) mediate the experiments. Emilie Bruyer left the group in May. Nain Mukesh joined the group in July. Gergő Thiering defended his PhD thesis in December. Next, we summarize our important achievements.

Biologists urgently need biomarker systems which trace e.g. cancer cells in the blood stream or provide fluorescent signals depending on the activity of neurons in brain. Such systems have been developed so far, but most of them are either unstable or toxic, thus they are not suitable for therapy. Our Semiconductor Nanostructures Research Group is, however, seeking such solutions that can be applied *in vivo*. Molecular-sized colloid SiC nanoparticles are very promising candidates to realize bioinert non-perturbative fluorescent nanoparticles for *in vivo* bioimaging. These SiC nanoparticles are prepared by wet chemical etching of large SiC particles. Our prepared colloid SiC nanoparticles are indeed fluorescent; however, the size dependence of the fluorescent properties were not understood. By advanced wet chemical etching methods, we were able to control the size of SiC nanoparticles and monitor their optical properties by steady-state and time-dependent optical methods. We found a direct evidence for transition from bulk-like to molecular-like fluorescence going from 4-6 nm to 2-4 nm sized SiC nanoparticles. Furthermore, we studied the interaction of molecular-sized SiC nanoparticles and BSA proteins as a model for human HSA proteins. By combining various optical techniques and simulation methods, the binding site of ultrasmall SiC nanoparticles to the BSA molecule was identified (see Fig. 1).

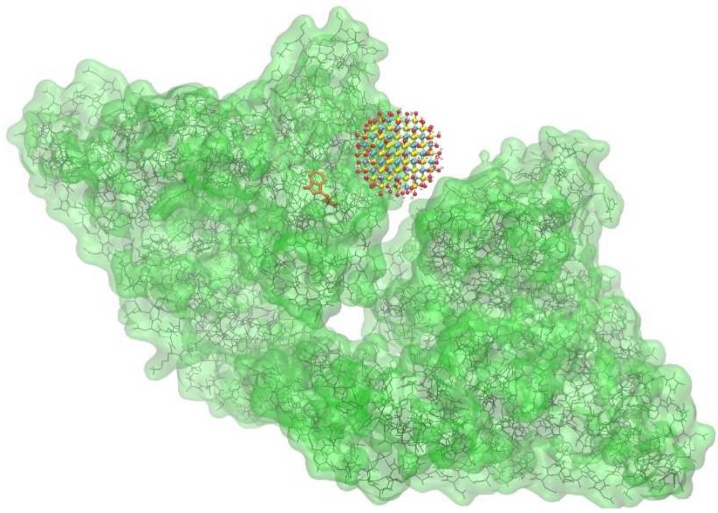

Figure 1. *Binding between BSA molecule (large greenish molecule) and ultrasmall silicon carbide nanoparticle (red and yellow balls and stick spherical structure).*

Significant results have been achieved in the research of solid-state quantum bits, which are the building blocks of a future implementation of the quantum computer. Diamond is a known host of solid-state qubits and single-photon emitters. Nitrogen-vacancy center (NV) stands out among these qubits in terms of robustness of optical spin readout and initialization. The microscopic mechanism behind the observed optical spin polarization was revealed by *ab initio* first-principles calculations. A new method was developed and implemented to describe the so-called highly-correlated electronic states in this and similar quantum bits that play a crucial role in the spin polarization process. Furthermore, the interaction between nearby NV quantum bit and acceptor defects was analyzed by the use of first-principles wavefunctions, and a novel mechanism for the decoherence of the quantum bit was revealed that may play an important role in the properties of near-surface NV quantum sensors. In addition, the ab initio magneto-optical spectrum of Group-IV--Vacancy color centers was calculated in diamond, and a new spin Hamiltonian was established in which the electron spin and the phonons are strongly coupled (see Fig. 2) that has an impact in the quantum communication applications of these quantum bits.

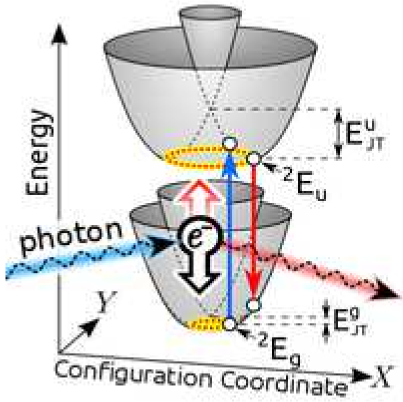

Figure 2. *Schematic diagram of the photoexcitation of the negatively charged Group-IV—vacancy color centers in diamond. The Jahn-Teller unstable ground state (^2E_g) state is photoexcited to the Jahn-Teller unstable excited state (^2E_u) by absorbing a photon, and emits a red-shifted photon in the decay process. The so-called Jahn-Teller energy (E_{JT}) in the corresponding states is also depicted.*

Furthermore, we studied nanosystems that are promising in biomarker and solar cell applications. The silicon nanoparticles (Si NPs) are very promising in various emerging technologies and for fundamental quantum studies of semiconductor nanocrystals. Heavily boron and phosphorus co-doped fluorescent Si NPs can be fabricated with diameters of a few nanometers. However, very little is understood about the structure and origin of the vibration and optical spectra of these NPs. By means of first-principles simulations, various spectroscopic quantities can be computed and compared to the corresponding experimental data. We characterized the size-dependent photoluminescence and Raman spectra of dopant-free Si NPs and found good agreement with the experiments (see Fig. 3). Based on these encouraging results, we utilized the same methodology to study the Raman and PL spectra of 10 randomly generated, heavily co-doped Si NP models (where we have chosen stable dopant configurations), and found that the results are in good agreement with the experimental spectra. These results imply that we could identify the dopant configurations in small Si NPs that are responsible for the observed photoluminescence, infrared vibration and Raman spectra.

Grants

EU H2020 No. DLV-820394: Asteriqs- Advancing Science and Technology through diamond Quantum Sensing (Adam Gali, 2017-2021)

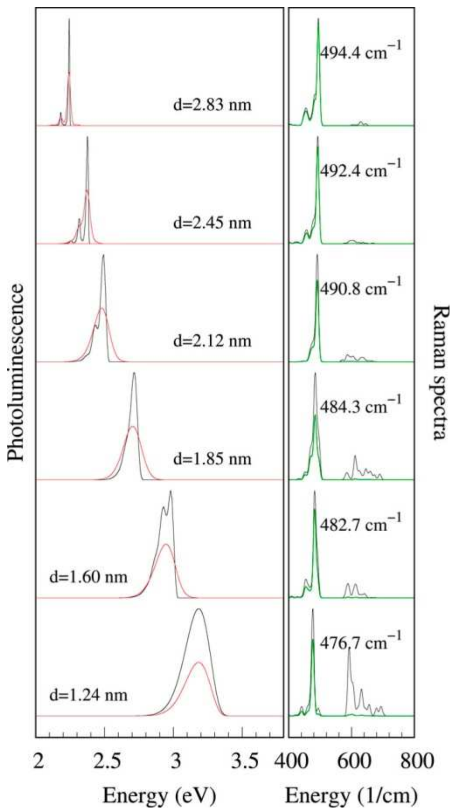

Figure 3. *The calculated photoluminescence emission spectra and resonant Raman spectra of hydrogen-terminated, pristine Si nanocrystals with diameters in the region of 1.1-2.8 nm. For the PL spectra, black and red curves correspond to 0 K and 300 K, respectively. For the Raman spectra, black curves correspond to the full spectra, while green curves correspond to the projected Raman spectra where the outermost layer of Si atoms and H atoms is excluded from the projection.*

NKFIH-NN-118161: JST V4: Nanophotonics with metal – group-IV-semiconductor nanocomposites: From single nanoobjects to functional ensembles (NaMSeN, A. Gali, 2016-2018)

NKFIH NVKP_16-1-2016-0152958: Development of fluorescent dyes and microscope for the treatment of epilepsy, (Femtonics Ltd., Wigner participant: A. Gali, 2017-2019)

NKFIH NKP-2017-1.2.1-NKP-2017-00001 National Quantumtechnology Program: Creation and distribution of quantum bits and development of quantum information networks (A. Gali, 2017-2021)

NKFIH-NN-127889: EU QuantERA project: Scalable Electrically Read Diamond Spin Qubit Technology for Single Molecule Imagers (A. Gali, 2018-2021)

NKFIH-127902: EU QuantERA project: Spin-based nanolytics - Turning today's quantum technology research frontier into tomorrow's diagnostic devices (A. Gali, 2018-2021)

International cooperation

Pontificia Universidad Católica de Chile (Santiago de Chile, Chile), Biophysics with color centers in diamond and related materials (J. R. Maze)

RMIT (Melbourne, Australia), Color centers in SiC nanoparticles for bioimaging (S. Castalletto)

University of Melbourne (Melbourne, Australia), Single-photon emitters in SiC devices (B.C. Johnson)

University of Pittsburgh (USA), Prof. W. J. Choyke experimental group, SiC (nano)particles

University of Linköping (Sweden), Prof. Erik Janzén experimental group, point defects in SiC

Harvard University (USA), Prof. Michael Lukin experimental group, defects for quantum computing

University of Chicago (USA), Prof. David D. Awschalom experimental group, SiC defects for quantum computing

University of Stuttgart (Germany), Prof. Jörg Wrachtrup experimental group, defects for quantum computing

University of Ulm (Germany), Prof. Fedor Jelezko experimental group, defects for quantum computing

Hasselt University (Belgium), Prof. Milos Nesladek experimental group, defects in diamond

Kaunas University of Technology (Lithuania), Dr. Audrius Alkauskas theoretician group, defects in diamond and SiC

University of Erlangen-Nürnberg (Germany), Dr. Michel Bockstedte theoretician group, defects in diamond and SiC

University of Kobe (Japan), Prof. Minoru Fujii experimental group, Si nanoparticles

Charles University (Czech Republic), Prof. Jan Valenta experimental group, Si nanoparticles

Slovakian Academy of Sciences (Slovakia), Prof. Ivan Štich theoretician group, quantum Monte Carlo methods in Si nanoparticles

Warsaw University of Technology (Poland), Prof. Romuald B. Beck experimental group, Si layers and devices

University of Mainz (Germany), Prof. Dmitrii Budker experimental group, diamond defects

University of Saarland (Germany), Prof. Christoph Becher experimental group, diamond defects

Racah Institute of Physics, The Hebrew University of Jerusalem (Israel), solid-state quantum bits (Alex Retzker)

National Institutes for Quantum and Radiological Science and Technology (Japan), solid-state quantum bits (Takeshi Ohshima)

Materials Modeling and Development Laboratory, National University of Science and Technology "MISIS," (Russia), solid-state quantum bits (Igor A. Abrikosov)

Institute for Experimental Physics II, Universität Leipzig, solid-state quantum bits (Jan Meijer)

Universität Wien (Vienna, Austria), Silicon carbide quantum bits (Michael Trupke)

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See also: S-C.22, S-Q.1

S-H. Partially ordered systems

Wigner Research Group

Tamás Börzsönyi, Ágnes Buka[E], Nándor Éber, Katalin Fodor-Csorba[A], Antal Jákli, István Jánossy[A], Dániel Nagy, Péter Salamon, Ellák Somfai, Tibor Tóth-Katona

Granular materials. — Flow, rheology and packing of granular materials.

The stationary flow field in a quasi-two-dimensional hopper (Fig. 1a) was investigated experimentally. The behavior of materials consisting of beads and elongated particles with various aspect ratios was compared. We show that while the vertical velocity in the flowing region can be fitted with a Gaussian function for beads, in the case of elongated grains the flowing channel is narrower and is bordered with a sharper velocity gradient (Fig. 1b). For this case, we quantify deviations from the Gaussian velocity profile. Relative velocity fluctuations are considerably larger and slower for elongated grains (Fig. 1c).

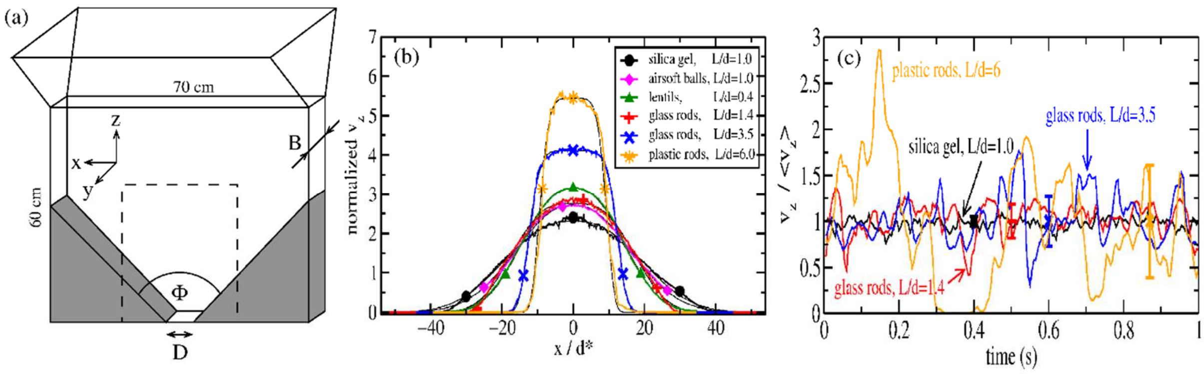

Figure 1. *(a) Sketch of the quasi-two-dimensional hopper, (b) vertical velocity across the hopper, (c) time evolution of the vertical velocity.*

The rheology of non-spherical granular particles has been investigated in inclined plane flows. Our discrete-element simulations and laboratory experiments revealed that density and friction are well-defined functions of the effective inertial number, which fully captures the effect of grain elongation.

We studied the packing of spheres experimentally and numerically in 2 + ε dimensions, realized by a container which is in one dimension slightly wider than the spheres. The particles organize themselves in a triangular lattice, while touching either the front or rear side of the container. This system appears to be similar to a frustrated spin-glass, but it has a well-defined ground state built up from isosceles triangles. When the system is agitated, it evolves very slowly towards the potential energy minimum through metastable states. We show that the dynamics is local and is driven by the optimization of the volumes of 7-particle configurations and by the vertical interaction between touching spheres.

Liquid crystals – We studied a stable lattice of topological defects appearing at the electric reorientation of a nematic fluid by quantitative polarimetry and by laser diffraction. The generation of optical vortices by topological defects was achieved and demonstrated in cases of two distinct mechanisms. First, individual defects convert circularly polarized light partially into a vortex beam with opposite handedness (Fig. 2a and 2b), while beams diffracted on the defect lattice do not carry vorticity. Second, dislocation of the lattice structure is a topological defect on a larger length scale; then beams diffracted on a single dislocation possess optical vortex character. For both cases, the vortex-generation efficiency is tunable by the applied voltage.

We studied the bending of liquid crystal membranes with phospholipids. The interactions of phospholipids with liquid crystals have formed the basis for attractive biosensor technologies. Phospholipids turn the liquid crystal director perpendicular to the LC/water interface. If the other side of the LC film is in contact with a surface that prefers perpendicular alignment, the LC film appears completely dark between crossed polarizers. Increasing the lipid concentration, the liquid crystal texture brightens again. We showed by optical surface profiler measurements (see Fig. 2) that the interface of the LC film suspended in a transmission electron microscopy (TEM) grid bends towards the lipid-coated interface. We demonstrated that where the bending occurs, the bent interface exhibits extreme sensitivity to air pressure variations, producing an optical response with acoustic stimulation. We suggested a physical mechanism for this result.

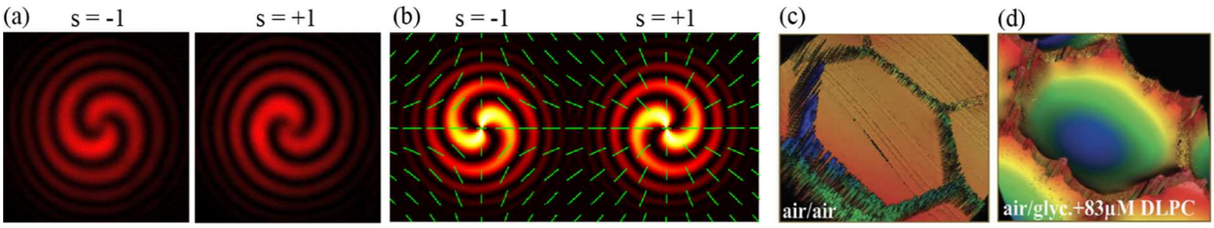

Figure 2. *Liquid crystal defect (with topological charge s =±1) generated optical vortices confirmed by interferometry: (a) experiments, (b) simulation. Liquid crystal membrane profiles with air on both sides (c) and with glycerol+pohospholipid on one side (d).*

The influence of UV light-induced pitch contraction and dilation on the electroconvection patterns (ECPs) of a chiral nematic liquid crystal containing a photoresponsive chiral dopant was investigated in planar-aligned cells. The helical twisting power of the dopant changed (even underwent handedness inversion) under UV irradiation; consequently, the pitch and the direction of the convection rolls in ECPs (being either parallel with or perpendicular to the surface alignment) could be controlled by the UV intensity and the ac voltage. The method of applying a light field allows a remote, contactless manipulation of the pitch, detectable via the morphological changes of ECPs, which can be utilized as a switchable optical grating.

In collaboration with German theoreticians, a concise theoretical description has been developed for the nonlinear regime of the dc electric field induced flexodomains of planar nematic liquid crystals. Experiments on different nematics demonstrated that the wave number increases almost linearly with the applied voltage. This behavior was confirmed by approximate analytical as well as precise numerical calculations.

Liquid crystal composite materials. — Magnetic-field-induced shift of the isotropic-to-nematic phase transition temperature has been measured in neat bent-core and calamitic liquid crystals (LCs), in their mixture, and in samples doped with spherical magnetic nanoparticles (i.e., in so called ferronematics – FNs) for two different orientations of the magnetic field. A magnetic-field-induced negative or positive shift of the transition temperature was detected depending on the magnetic field orientation with respect to the initial orientation of the nematic phase, and on the type of liquid crystal matrix as illustrated in Fig.3.

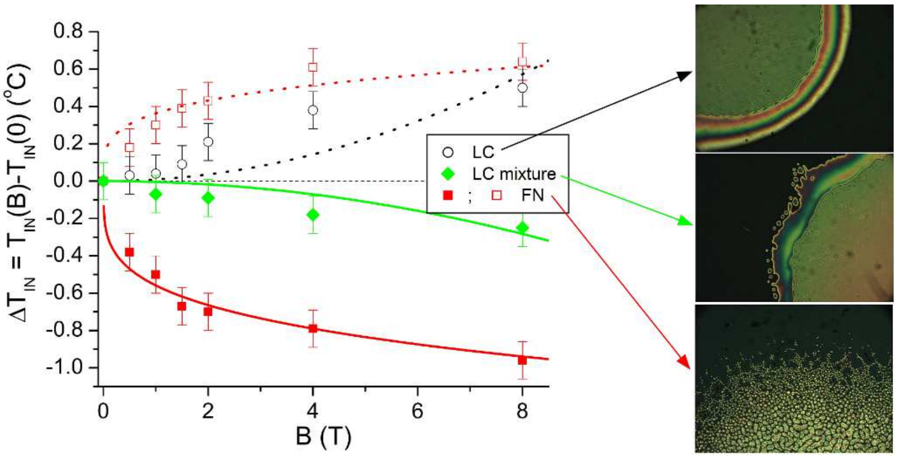

Figure 3. *Magnetic-field-induced phase transition temperature shifts detected in a calamitic liquid crystal (LC), in its mixture with a bent-core LC, and in a ferronematic (FN) based on them. The lines represent theoretical fits. On the right: microphotographs of the isotropic-to-nematic phase transition in these systems.*

Photo-sensitive mesogenic materials and surfaces. — In planar nematic liquid crystal cells, twist deformation was generated through photoalignment. By increasing the twist angle gradually, supertwisted cells were constructed in the range of 2π–3π twist angle. The supertwist relaxed through the formation of either π or 2π inversion loops, depending on the character of the photosensitive substrate. The difference in the relaxation process was related to the zenithal anchoring strength on the photosensitive plate.

Magneto-sensitive surfaces. — We investigated the surface topographical modifications of a soft magnetoactive elastomer in response to magnetic fields. Optical profilometry analysis showed that the magnetic field-induced surface roughness with respect to magnetic field is in the range of 1 mm/T. Sessile water droplet shape analysis revealed that the field-induced topographical modifications affect the contact angle at the surface. This effect is reversible and the responsivity to magnetic field was found in the range of 20°/T. Despite the increased surface roughness, the apparent contact angle decreases with increasing field, which is attributed to the field-induced protrusion of hydrophilic microparticles from the surface layer.

Grants

NKFIH K 116036: Flow and rheology of non-spherical particles (E. Somfai, 2016-2020)

NKFIH FK 125134: Tunable topology of confined soft matter (P. Salamon, 2017-2021)

NKFIH PD16 121019: Interfacial topology of anisotropic soft matter, (P. Salamon, 2016-2019)

International cooperation

COST Action CA17139: European Topology Interdisciplinary Action, (Management Committee Member: P. Salamon, 2018-2022)

Otto-von-Guericke Universitaet Magdeburg (Germany): Multiparticle systems with complex interactions: effects of particle surface, shape and deformability (T. Börzsönyi, 2018-2019)

Ecole Supérieure de Physique et de Chimie Industrielles de Paris (France): joint PhD supervision (T. Börzsönyi, 2018-2021)

RIKEN (Wako, Japan): Creation, active control, and possible application of topological defects in advanced soft matter systems (Á. Buka, 2016-2018)

Jožef Stefan Institute (Ljubljana, Slovenia): Microfluidic systems based on anisotropic soft matter (P. Salamon, 2016-2018)

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S-J. Gas discharge physics

Wigner reseach group

Kinga Kutasi, Aranka Derzsi, Zoltán Donkó, Péter Hartmann, Péter Magyar[#], Pál Mezei[A]

Gas discharge physics. — We developed a particle-based simulation code for the description of short-pulsed (~ns) discharges at atmospheric-pressure helium gas with an admixture of molecular nitrogen (at concentrations ≤1%). In this code, we have also included the photon treatment of the VUV resonance radiation of helium. We have explored the spatiotemporal evolution of charged species densities, reaction rates, and the fluxes of ”active” species at the surfaces. We have investigated, as well, the behaviour of the electron velocity distribution function and the electron energy probability function, and concluded that these deviate significantly from the Maxwell-Boltzmann distribution, especially in the cathode region of the discharge. These observations demonstrated the usefulness (and uniqueness) of particle simulations of similar physical systems. We have found that the VUV resonance radiation of He-atoms is heavily trapped within the high-pressure gaseous environment and photons are absorbed/re-emitted typically several hundred times before leaving the plasma. Nonetheless, the escaping photons were found to contribute significantly to the electron emission process at the electrodes. For most conditions studied, an increase of around a factor of two of the current pulse peak was observed when VUV photons were included in the simulations, in comparison to those cases when their effect was neglected. Fig. 1 shows results for a plane-parallel electrode configuration with a gap of 1 mm, to which a high voltage pulse with an amplitude of 1000 V is applied with a trapezoidal shape. Current pulses in the order of 10 A are generated over the electrode surface of 1 cm^2, when VUV photons are not considered in the simulation (at an initial charged particle density of 1.5×10^{11} cm^{-3}). The peak current grows to ~20 A, when VUV photons are included. The figure also shows the time integrated wavelength-resolved radiation from the plasma, in the vicinity of the theoretical wavelength of the $2^1P \rightarrow 1^1S$ resonant transition.

We have performed systematic investigation of the influence of various surface processes - such as the secondary electron (SE) emission induced by ions and electrons, and electron reflection at the electrodes - on the discharge characteristics in low-pressure, capacitively coupled radiofrequency discharges. By using a realistic (energy-dependent) model for the description of the electron-surface interaction in our Particle-in-Cell/Monte-Carlo Collisions (PIC/MCC) simulation code, we have studied the effect of the electron-induced SEs on the discharge characteristics in the 0.5 Pa–3 Pa pressure range, for voltage amplitudes between 100 V–1500 V, assuming different SE yields for ions (γ–coefficient). Such discharge conditions are typical in industrial applications, such as plasma etching, sputtering and plasma-immersion ion implantation. We demonstrated that the realistic description of the electron-surface interaction significantly alters the computed plasma parameters, compared to results obtained based on a simple model (which completely neglects the emission of SEs due to electron impact) for the description of the electron-surface interaction, widely used in PIC/MCC simulations of low-pressure capacitively coupled plasmas.

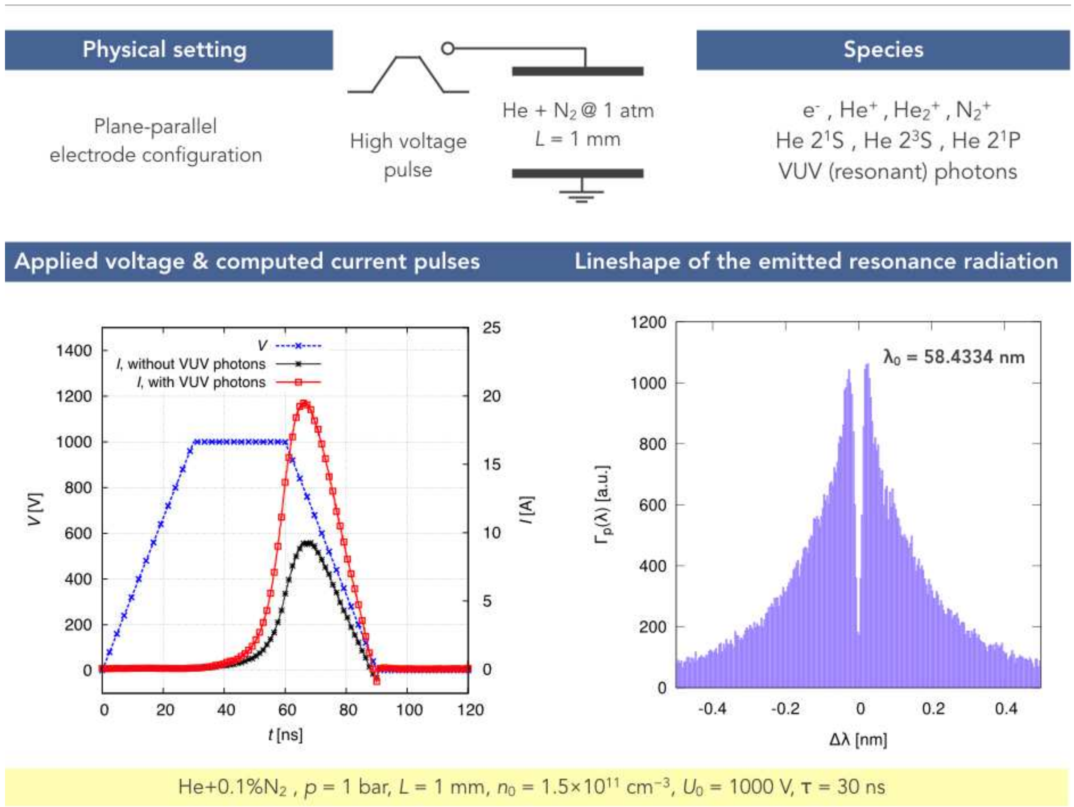

Figure 1. *Physical setting, simulated species, parameter values, and results of the numerical studies of nanosecond discharges (applied voltage and computed discharge current waveforms, as well as the lineshape of the He resonance radiation).*

We have found that both the gas pressure and the value of the γ-coefficient affect the role of electron induced SEs (δ-electrons) in shaping the discharge characteristics at different voltage amplitudes. Their effect on the ionization dynamics has been found to be most striking at low pressures, high voltage amplitudes and high values of the γ-coefficient (see Fig. 2). At low pressures, the energetic ion-induced SEs (γ -electrons) generated at one electrode and accelerated towards the bulk by the local sheath electric field, can cross the bulk without

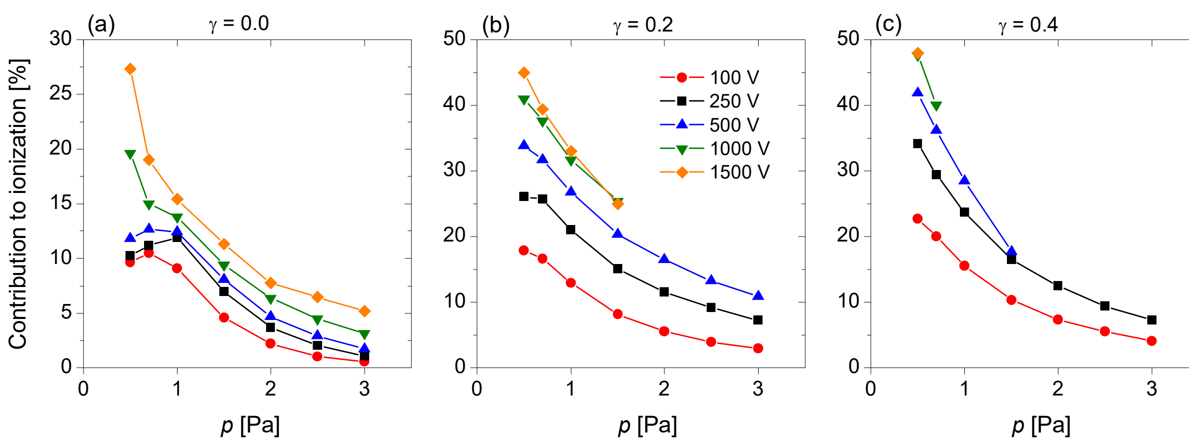

Figure 2. *Contribution of electron-induced secondary electrons (δ-electrons) to the total ionization at different pressures and voltage amplitudes for different values of the ion-induced secondary electron emission coefficent, γ.*

collisions and generate a high number of electron-induced SEs (δ-electrons) upon their impact at the opposite electrode. Depending on the instantaneous local sheath voltage, these δ-electrons are accelerated into the plasma bulk, where they generate significant ionization and enhancement of the plasma density. On the other hand, at high pressures due to the more frequent collisions, the electrons reach the electrodes at lower energies, which leads to a decrease of the number of SEs emitted by electron impact at the electrodes, therefore, to a decrease of the contribution of δ-electrons to the ionization.

Dusty plasmas. — In the field of dusty plasma physics, we have realized a rotating electrode experiment to measure the diffusion of highly charged dust particles in large external quasi-magnetic field. We have shown that with increasing magnetization, the transport becomes hindered and the non-Maxwellian nature becomes more prominent as strong super-diffusion is observed. Our experimental results are supported by molecular dynamics simulations of magnetized Yukawa systems. In relation to the PK-4 dusty plasma experiment onboard the International Space Station (ISS), we have implemented a cylindrical 2D particle-in-cell with Monte Carlo collisions (PIC/MCC) numerical simulation for direct-current neon discharges. Our results indicate that the apparently quiet positive column as observed in the experiment with long exposure time imaging is in fact made of quickly moving ionization waves, as shown in Fig. 3. Our numerical prediction has been confirmed by fast camera imaging experiments. The presence of ionization waves explains the unexpected observation of dominant dust particle chain formation in the micro-gravity setup.

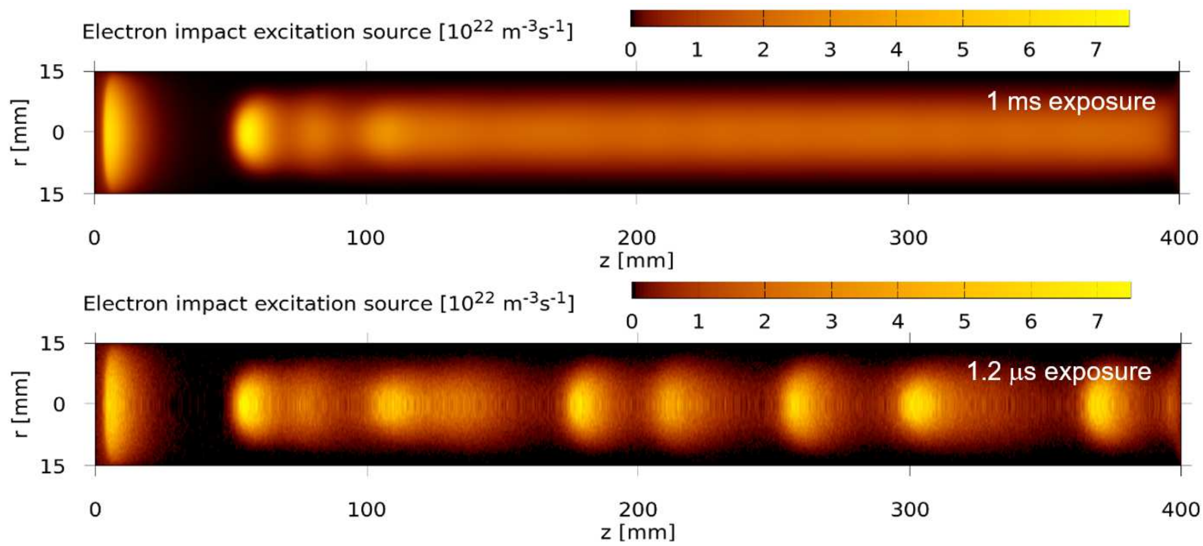

Figure 3. *Electron impact excitation source from the PK-4 neon discharge simulation at long and short exposure times.*

Reactive plasmas. — In the last decade, plasma-activated water (PAW), or, more generally, plasma-activated liquid (PAL) has received a lot of attention from the plasma medicine and plasma agriculture community due to its potential to induce oxidative stress to cells. By PAL it is meant the liquid which contains reactive species, mostly reactive oxygen and nitrogen species (RONS) generated by the interaction of active or afterglow plasma with the liquid. PAW has been found to have antimicrobial and antibacterial effect, which is thought to occur due to the synergetic effect between the RONS and/or pH of the solution. Plasma activated buffered solution and cell culture media have also been studied for therapeutical aims, and its potentials for cancer therapy have also been shown. In the field of agriculture with PAW, the improvement of seeds germination and plant growth have been targeted. The main long-lived RONS produced in PAL have been identified to be H_2O_2, NO_2^- and NO_3^-. The usual studies report typically one or two PAL conditions, giving no further suggestions for PAL composition tuning. In order to be able to identify the role of different species and to clarify the synergy effects in the interaction of PAL with biological systems, PAL with different compositions would be welcomed, in what concerns the density ratios of different RONS.

With our study we have shown the possibility of tuning the ratio of active species concentrations over three orders of magnitude in deionized water (DIW) activated with a surface-wave microwave discharge (see Fig. 4) by varying the gas flow rate, initial gas mixture composition and treatment distance. The surface-wave microwave discharge is generated with the help of a surfatron launcher in a quartz tube of outer diameter 6 mm and inner diameter 4 mm using as a main gas Ar at gas flow rates of 1500 and 2000 sccm (Ar_x conditions in Figure 4). Ar-N_2/O_2 binary (ArN_2_x and ArO_2_x conditions) and ternary (ArN_2O_2_x conditions) mixtures are also used with the O_2 and N_2 gas flow rates ranging between 10-100 sccm. The input power is varied between 25 and 30 W, and the DIW is positioned below the plasma plume with the water surface being at d = 5.5 - 10.5 mm distance from the edge of the quartz tube, see Fig. 5. By changing the mixture composition and the treatment distance, at the plume - water surface interaction point the electron density is changed, which determines the concentration of H_2O_2 created in the liquid phase.

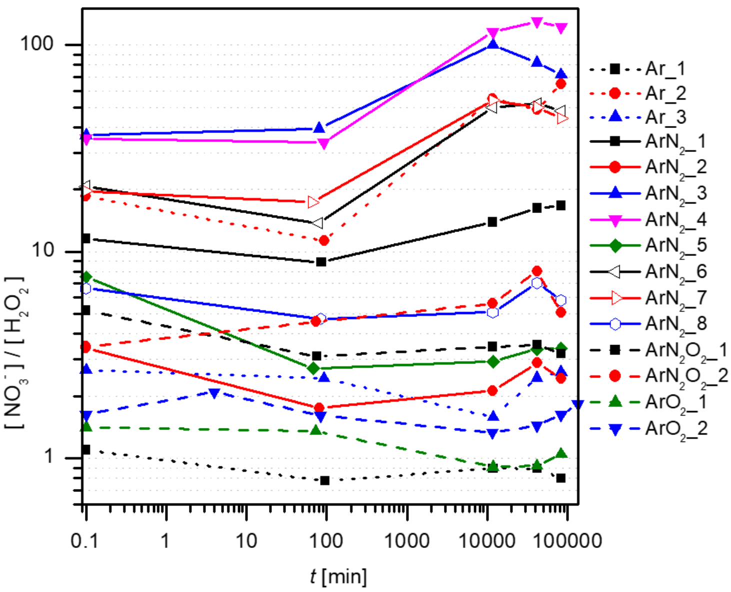

Figure 4. *The ageing of the nitrate to hydrogen peroxide concentration ratio in the case of PAWs produced by Ar/N_2/O_2 surface-wave microwave discharges at different discharge and treatment conditions.*

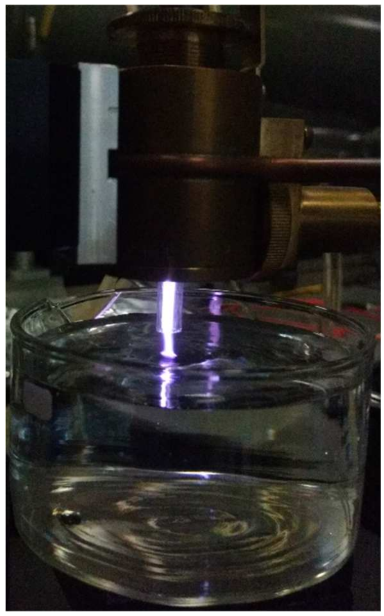

Figure 5. *A surface-wave microwave discharge in interaction with water surface.*

Grants:

NKFIH K-119357 Non-equilibrium charged particle kinetics in ionized gases (Z. Donkó, 2016-2020)

NKFIH PD-121033 Reactive gas discharges excited by tailored voltage waveforms (A. Derzsi, 2016-2019)

NKFIH K-115805 Complex plasmas in action (P. Hartmann, 2015-2019.08.31)

NKFIH FK-128924 Control of ion properties in low-pressure radiofrequency gas discharges relevant for surface processing (A. Derzsi, 2018-2022)

Bilateral HAS – Serbian Academy of Sciences Interaction of non-equilibrium atmospheric pressure plasmas with model surfaces (K. Kutasi, 2016-2018)

TÉT_16-1-2016-0014 New technologies in agriculture based on cold gas discharge plasmas (Hungarian-Croatian Intergovernmental project, K. Kutasi, 2017-2019)

International cooperation

Boston College, MA, USA (G. J. Kalman)

Univ. Kiel, Germany (M. Bonitz)

West Virgina University, USA (J. Schulze)

Ruhr University, Bochum, Germany (R.P. Brinkmann, J. Schulze)

Brandenburg University of Technology, Cottbus, Germany (T. Mussenbrock)

Ecole Polytechnique, Paris, France (J.-P. Booth)

Baylor University, Waco, TX, USA (Truell W. Hyde)

University of California San Diego, La Jolla, CA, USA (M. Rosenberg)

University of York, UK (Deborah O'Connell, Timo Gans)

Institute of Physics Belgrade (Belgrade, Serbia), Interaction of discharge plasmas with surfaces (Zoran Lj. Petrovic, Nevena Puac)

Josef Stefan Institute Ljubljana (Ljubljana, Slovenia), Surface treatments in afterglow plasmas (Miran Mozetic)

Institut Jean Lamour Ecole des Mines Nancy (Nancy, France), Gabriel Lippmann Centre Luxembourg (Luxembourg) Elementary processes in afterglow plasmas (Thierry Belmonte, David Duday)

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S-P. Ultrafast, high-intensity light–matter interactions

"Momentum" Research Team

Péter Dombi, Balázs Bódi[#], Viktória Csajbók[#], Győző Farkas[E], Norbert Kroó[E], Benedek Nagy[#], Zsuzsanna Pápa, Péter Rácz, Péter Sándor

Strong-field interactions and nano-optics experiments. — Probing nanooptical near-fields is a major challenge in plasmonics. We demonstrated an experimental method based on utilizing ultrafast photoemission from plasmonic nanostructures that is capable of probing the maximum nanoplasmonic field enhancement in any metallic surface environment. Directly measured maximum field enhancement values for various samples are in good agreement with detailed finite-difference time-domain simulations. These results established ultrafast plasmonic photoelectrons as versatile probes for nanoplasmonic near-fields. We extended this method to probe the evolution of plasmonic near-fields on few-femtosecond time-scales, representing the natural time-scale of the buildup and decay of collective electron oscillations by light. Fig. 1 shows the scheme and results of these experiments.

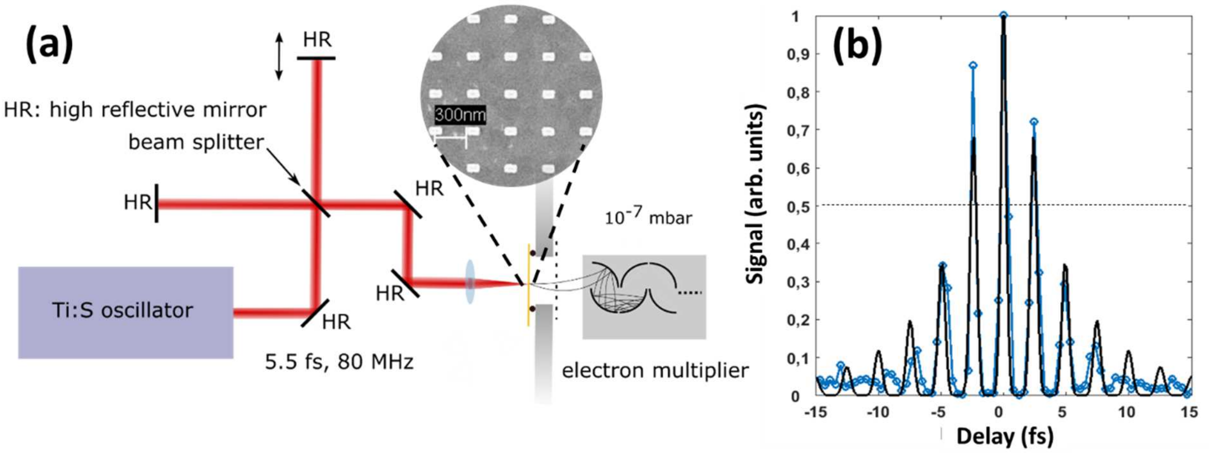

Figure 1. *(a) The output of an interferometric autocorrelator setup illuminated by 5.5-fs laser pulses is focused onto a substrate with plasmonic nanoparticles. Photoelectron spectra are recorded in vacuum. (b) Measured (blue) and reconstructed (black) third-order interferometric autocorrelation curves of the few-femtosecond plasmonic near-field.*

In addition, we used this method to probe the coupling between propagating and localized surface plasmon modes, a fundamental question in plasmonics.

Laser fusion enhanced by metal nanoparticles. — Localized surface plasmon assisted laser fusion was also studied, where achieving the needed high temperature for ignition could be realized not by compression, but by direct heating. This can be achieved by putting into the target plasmonic nanorods or nanoshells. „Time-like" implosion of the total target volume may be realized by proper distribution of the nanoparticles in the target volume. Shorter (picosecond instead of nanosecond) laser pulses, smaller and flat samples and only 2 laser beams (hitting the target from opposite directions) may be used and a few times 10 Joule energy pulses may already lead to implosion.

Femtosecond photonics. — Improving the laser-induced damage threshold of optical components is a basic endeavor in femtosecond technology. By testing more than 30 different femtosecond mirrors with 42 fs laser pulses at 1 kHz repetition rate, we found that a combination of high-bandgap dielectric materials and improved design and coating techniques enable femtosecond multilayer damage thresholds exceeding 2 J/cm^2 in some cases. We also studied damage threshold as a function of the number of interacting pulses and other relevant parameters.

Ultrashort laser pulses provide an excellent dry and clean patterning technique in nanoscience for preparing quantum dots and quantum wires as well as depositing nanocrystalline grains of technologically important semiconductors. We experimentally demonstrated the formation of silicon carbide (SiC) nanocrystals with wide size distribution (70–700 nm) by irradiation of carbon layers deposited on silicon wafers with ultrashort laser pulses of 42 fs pulse duration with 1 kHz repetition rate. Surface morphology of the laser-irradiated region monitored by scanning electron microscopy (SEM) exhibits nanocrystalline agglomerates of various size in the vicinity of ablated craters. Transmission electron microscopy (TEM) measurements show the occurrence of ~ 100 nm size cubic and hexagonal SiC polytypes in addition to Si and amorphous silica nanoparticles. Further development of this laser-induced process and the accurate control of the laser pulse parameters can open new routes for preparing tailor-made SiC nanomaterials that have useful properties for electronic and biomedical applications.

Grants

"Momentum" Program of the HAS (P. Dombi, 2014-2019)

Max Planck Society Partner Group Grant: Ultrafast strong-field nanoplasmonics (P. Dombi, 2014-2019)

VEKOP Grant: Research on ultrahigh-speed molecular and nanooptical switches (P. Dombi, G. Vankó, 2017-2021)

OTKA K-109257: Time-resolved investigations of functional molecules and metal nanoparticles (P. Dombi, 2014-2018)

OTKA 125249: Ultrafast processes in nanooptics (P. Rácz, 2017-2021)

OTKA 128077: Femtosecond plasmon dynamics in nansystems (Z. Pápa, 2018-2022)

International cooperations

Max Planck Institute of Quantum Optics (Garching, Germany) with P. Dombi.

Carl von Ossietzky University (Oldenburg, Germany) with P. Dombi and B. Nagy.

Texas A&M University (College Station, USA) with N. Kroó.

University of Ulm (Germany) with N. Kroó.

University of Graz (Austria) with P. Dombi.

Publications

Articles

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4. Nayak A, Orfanos I, Makos I, Dumergue M, Kuhn S, Skantzakis E, Bódi B, Varju K, Kalpouzos C, Banks HIB, Emmanouilidou A, Charalambidis D, Tzallas P: Multiple ionization of argon via multi-XUV-photon absorption induced by 20-GW high-order harmonic laser pulses. ***PHYS REV A*** **98**:2 023426/1-8 (2018)
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See also: R-L.2, S-R.5

S-S. Quantum optics

"Momentum" Research Team

Péter Domokos, Thomas W. Clark, András Dombi, Dávid Jakab[#], Gábor Kónya[#], Dávid Nagy, Gergely Szirmai, András Vukics, F. I. B. Williams

Experiment on Cavity Quantum Electrodynamics with cold Rb atoms. — We set up a new laboratory for cavity QED experiments with ultracold Rb atoms (Fig. 1). We realized the UHV system which is operated in the pressure range below 10^{-10} mbar, and includes the magneto-optical trap and the in-vacuo high-finesse single-mode optical resonator. We completed the optical system, which is based on three laser sources that are referenced to Rb resonance line by Doppler-free non-linear spectroscopy. By means of acousto-optical modulators, we provide the narrow-linewidth phase-locked laser sources at five different frequencies for atomic manipulation.

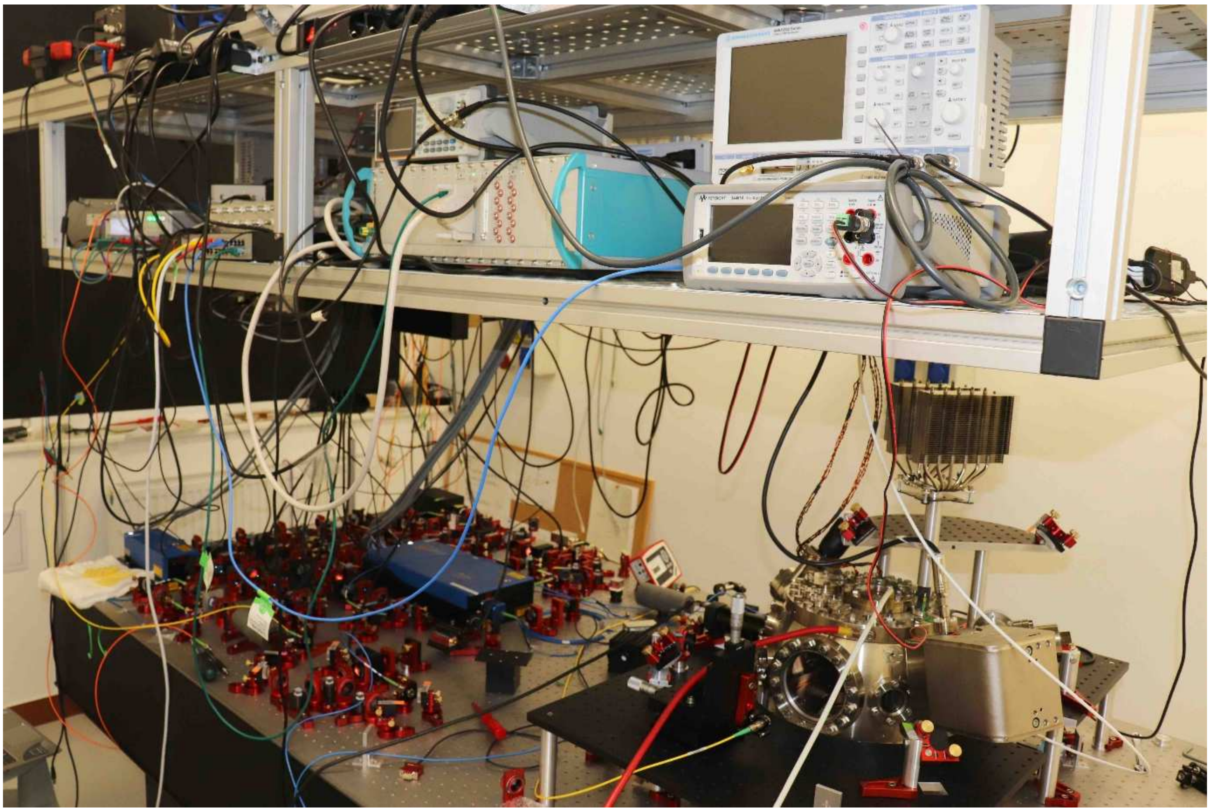

Figure 1. *Photo of the actual status of the cavity QED laboratory.*

Cavity Quantum Electrodynamics, quantum critical phenomena. — The quantum measurement back-action noise effects on the dynamics of an atomic Bose lattice gas inside an optical resonator have been described by means of a hybrid model consisting of a Bose–Hubbard Hamiltonian for the atoms and a Heisenberg–Langevin equation for the lossy cavity field mode (Fig. 2). Considering atoms initially prepared in the ground state of the lattice Hamiltonian, we calculated the transient dynamics due to the interaction with the cavity mode. We showed that the cavity field fluctuations originating from the dissipative outcoupling of photons from the resonator lead to vastly different effects in the different possible ground state phases, i.e., the superfluid, the supersolid, the Mott- and the charge-density-wave phases. In the former two phases with the presence of a superfluid wavefunction, the quantum measurement noise appears as a driving term leading to depletion of the ground state. The time scale for the system to leave the ground state was presented in a simple analytical form. For the latter two incompressible phases, the quantum noise results in the fluctuation of the chemical potential. We derived an analytical expression for the corresponding broadening of the quasiparticle resonances.

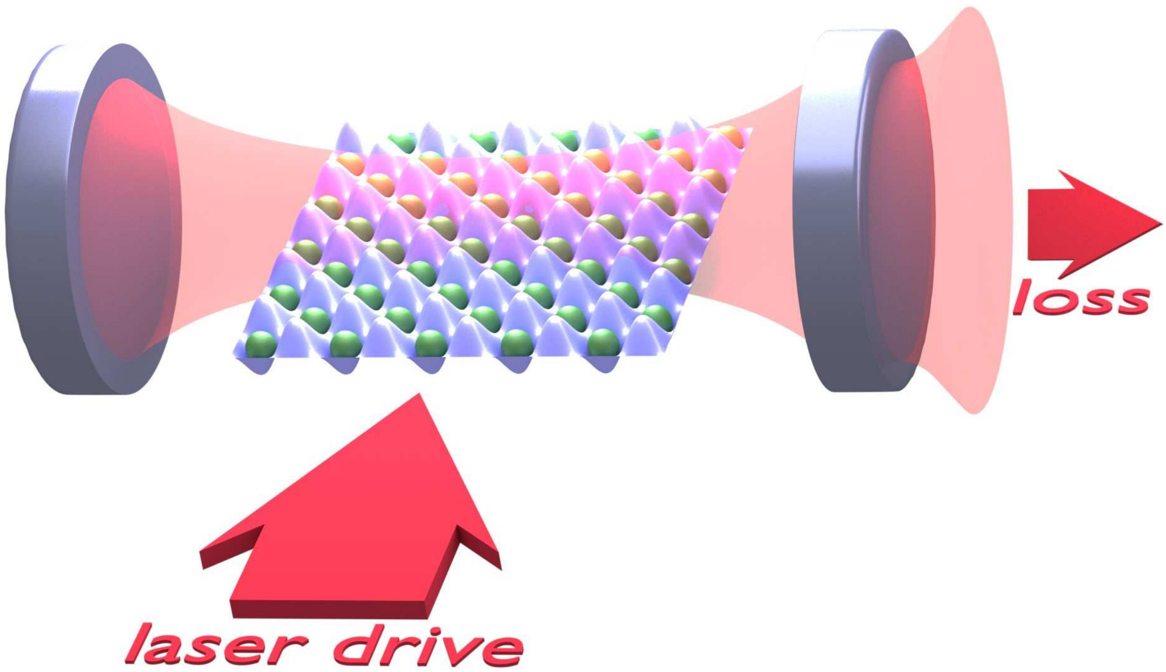

Figure 2. *Illustration of the coupled cavity Bose-Hubbard model setup. An atomic cloud is loaded into a square optical lattice, which is inside a single-mode high-Q Fabry-Pérot resonator. The period of the cavity mode is approximately equal to that of the optical lattice. The cavity is pumped from the side by light scattering off the atoms. The system is open: together with the external drive, the photons leak out from the cavity, resulting in heating and decoherence, or, in other terms, quantum measurement back-action since the out-coupled photons can be measured by classical detectors.*

Ultracold gases, Bose-Einstein condensates. — We studied quasiparticle scattering effects on the dynamics of a homogeneous Bose-Einstein condensate of ultracold atoms coupled to a single mode of an optical cavity. The relevant excitations, which are polariton-like mixed excitations of photonic and atomic density-wave modes, have been identified. All the first-order correlation functions were presented by means of the Keldysh Green's function technique. Beyond confirming the existence of the resonant enhancement of Beliaev damping, we found a very structured spectrum of fluctuations. There is a spectral hole burning at half of the recoil frequency, reflecting the singularity of the Beliaev scattering process. The effects of the photon-loss dissipation channel and that of the Beliaev damping due to atom-atom collisions could be well separated. We showed that the Beliaev process does not influence the properties of the self-organization criticality.

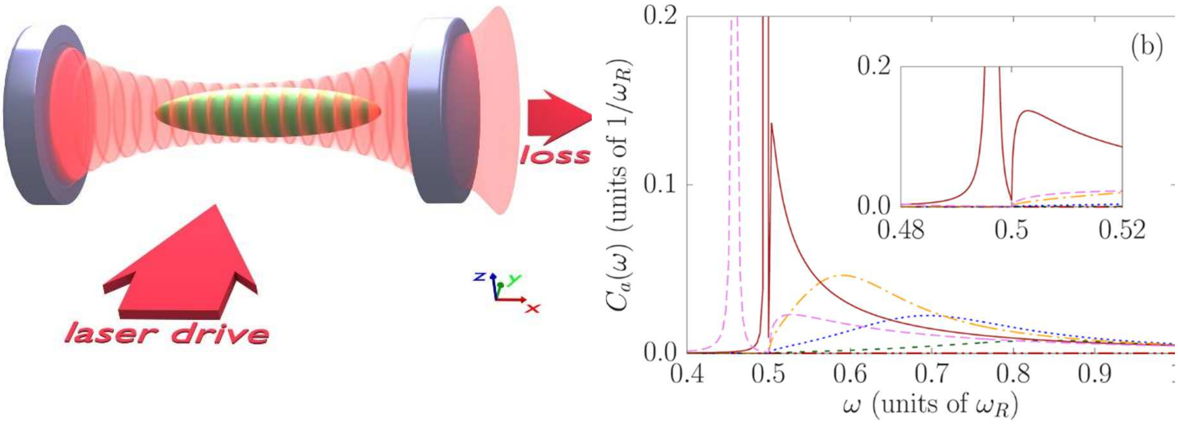

***Figure 3**. (a) The schematic picture of an atomic ensemble inside a Fabry-Pérot cavity pumped from the side by a laser close to resonance with the cavity. The atomic gas undergoes self-organization for strong enough laser drive: the atoms scatter photons from the laser to the cavity and may create a classical field serving as an optical lattice trapping them even further in the optimal scattering positions. (b) Spectrum of the quasiparticle excitation. Large detuning $\Delta C = 100$ implies little mixing of the condensate quasiparticle with the photon mode. The enhanced Beliaev scattering process is manifested by the large peak, which exhibits a hole burning at 0.5. (All angular frequencies are expressed in units of the recoil frequency.) The correlation function is plotted for different coupling strengths y approaching the critical value y_c: $y = 0$ (solid red), $y/y_c = 0.5$ (short-dashed green), 0.7 (dotted blue), 0.8 (dash-dotted orange), 0.9 (dashed-double-dotted brown), 0.95 (long-dashed magenta).*

We studied the spin-1 bilinear–biquadratic model on the complete graph of N sites, i.e. when each spin is interacting with every other spin with the same strength. Because of its complete permutation invariance, this Hamiltonian can be rewritten as the linear combination of the quadratic Casimir operators SU(3) and SU(2). Using group representation theory, we explicitly diagonalized the Hamiltonian and mapped out the ground-state phase diagram of the model. Furthermore, the complete energy spectrum with degeneracies was obtained analytically for any number of sites.

Grants

“Momentum” Program of the HAS Quantum Measurement Theory in Hybrid Mesoscopic Couplers and Networks (P. Domokos)

National Excellence Program for Quantum Technology, HunQuTech Consortium: Preparation, distribution of quantum bits and development of quantum information networks (2017-1.2.1-NKP-2017-00001, 2017-2021)

OTKA K-115624: Open quantum system dynamics in the ultrastrong coupling regime (P. Domokos, 2015-2019)

International cooperation

Fortágh group, Physikalisches Institut, Eberhard-Karls-Universität Tübingen, D-72076 Tübingen, Germany

Johannes Fink, Institute of Science and Technology Austria, 3400 Klosterneuburg, Austria

Wallraff group, Department of Physics, ETH Zürich, CH-8093 Zürich, Switzerland

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S-T. Quantum information and foundations of quantum mechanics

Wigner Research Group

Tamás Kiss, János Asbóth, Péter Ádám, Péter Boross, Aurél Gábris[A], Orsolya Kálmán, Zsolt Kis, Miklós Kornyik[#], Pavlo Pyshkin, Viktor Szalay, Géza Tóth[A]

Measurement-induced nonlinear transformations. — We considered the task of deciding whether an unknown qubit state falls in a prescribed neighborhood of a reference state. If several copies of the unknown state are given and we can apply a unitary operation pairwise on them combined with a postselection scheme conditioned on the measurement result obtained on one of the qubits of the pair, the resulting transformation is a deterministic, nonlinear, chaotic map in the Hilbert space. We derived a class of these transformations which are capable of orthogonalizing nonorthogonal qubit states after a few iterations. These nonlinear maps orthogonalize states, which correspond to the two different convergence regions of the nonlinear map. Based on the analysis of the border (the so-called Julia set) between the two regions of convergence, we showed that it is always possible to find a map capable of deciding whether an unknown state is within a neighborhood of fixed radius around a desired quantum state. We analyzed which one- and two-qubit operations would physically realize the scheme. It is possible to find a single two-qubit unitary gate for each map or, alternatively, a universal special two-qubit gate together with single-qubit gates in order to carry out the task. We note that it is enough to have a single physical realization of the required gates due to the iterative nature of the scheme.

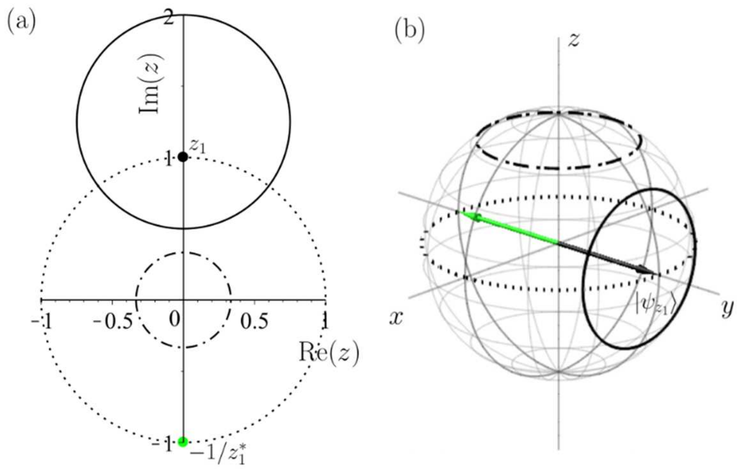

Figure 1. *The decomposition of the relevant map f into the subsequent actions of a contracting two-qubit operation and a single-qubit unitary operation.*

(a) The effect of the decomposition on the complex plane (projection of the Bloch sphere), representing the initial states of the qubit. States within the solid circle are matched.

(b) The same decomposition represented on the Bloch sphere.

Quantum walks — Measurements on a quantum particle unavoidably affect its state, since the otherwise unitary evolution of the system is interrupted by a nonunitary projection operation. To probe measurement-induced effects in the state dynamics using a quantum simulator, the challenge is to implement controlled measurements on a small subspace of the system and continue the evolution from the complementary subspace. A powerful platform for versatile quantum evolution is represented by photonic quantum walks because of their high control over all relevant parameters. However, measurement-induced dynamics in such a platform have not yet been realized. We participated (at the University of Paderborn) in the implementation of controlled measurements in a discrete-time quantum walk based on time-multiplexing. This was achieved by adding a deterministic outcoupling of the optical signal to include measurements constrained to specific positions resulting in the projection of the walker's state on the remaining ones (Fig. 2). With this platform and coherent input light, we experimentally simulated measurement-induced single-particle quantum dynamics. We demonstrated the difference between dynamics with only a single measurement at the final step and those including measurements during the evolution. To this aim, we studied recurrence as a figure of merit, that is, the return probability to the walker's starting position, which was measured in the two cases. We tracked the development of the return probability over 36 time steps and observed the onset of both recurrent and transient evolution as an effect of the different measurement schemes, a signature that only emerges for quantum systems. Our simulation of the observed one-particle conditional quantum dynamics does not require a genuine quantum particle but was demonstrated with coherent light.

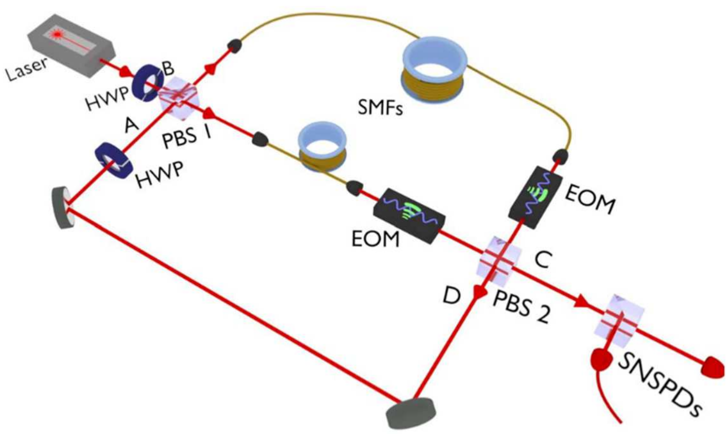

***Figure 2.** Schematic of the experimental setup of the time-multiplexed quantum walk with active in- and outcoupling realized by two EOMs (electro-optical modulators). The active control of the switches allows to implement in the time domain both the continual and reset measurement schemes. HWP, half-wave plate; PBS, polarizing beam splitter; SMF, single-mode fiber; SNSPDs, superconducting nanowire single-photon detectors.*

Rotational-vibrational quantum states in molecules. — We determined the internal-axis system (IAS) of molecules with a large amplitude internal motion (LAM) by integrating the kinematic equation of the IAS by Lie-group and Lie-algebraic methods. Numerical examples on hydrogen peroxide, nitrous acid, and acetaldehyde demonstrate the methods. By exploiting the special product structure of the solution matrix, we devised simple methods for calculating the transformation to the rho-axis system (RAS) along with the value of the parameter ρ characterizing a RAS rotational-LAM kinetic energy operator. The parameter ρ so calculated agrees exactly with that one obtained by the Floquet method as shown in the example of acetaldehyde. We gave geometrical interpretation of ρ. We numerically demonstated the advantageous property of the RAS over the IAS in retaining simple periodic boundary conditions.

Nanophotonics. — Non-linear second-harmonic wave generation (SHG) has been thoroughly examined in one dimension both analytically and numerically. Recently, the application of advanced domain poling techniques enabled the fabrication of two-dimensional (2D) patterns of the sign of the nonlinear coefficient in certain non-linear crystals, such as $LiNbO_3$ and $LiTaO_3$. This method can be used to achieve quasi-phase-matching in SHG and hence amplification of the second harmonic fields in 2D. We have worked out a true vectorial numerical method for the simulation of SHG by extending the finite-difference frequency-domain method (FDFD). Our nonlinear method (NL-FDFD) operates directly on the electromagnetic fields, uses two meshes for the simulation (for ω and 2ω fields), and handles the non-linear coupling as an interaction between the two meshes. Final field distributions can be obtained by a small number of iteration steps. NL-FDFD can be applied in arbitrarily structured linear media with an arbitrarily structured χ^(2) component both in the small conversion efficiency and the pump-depleted cases.

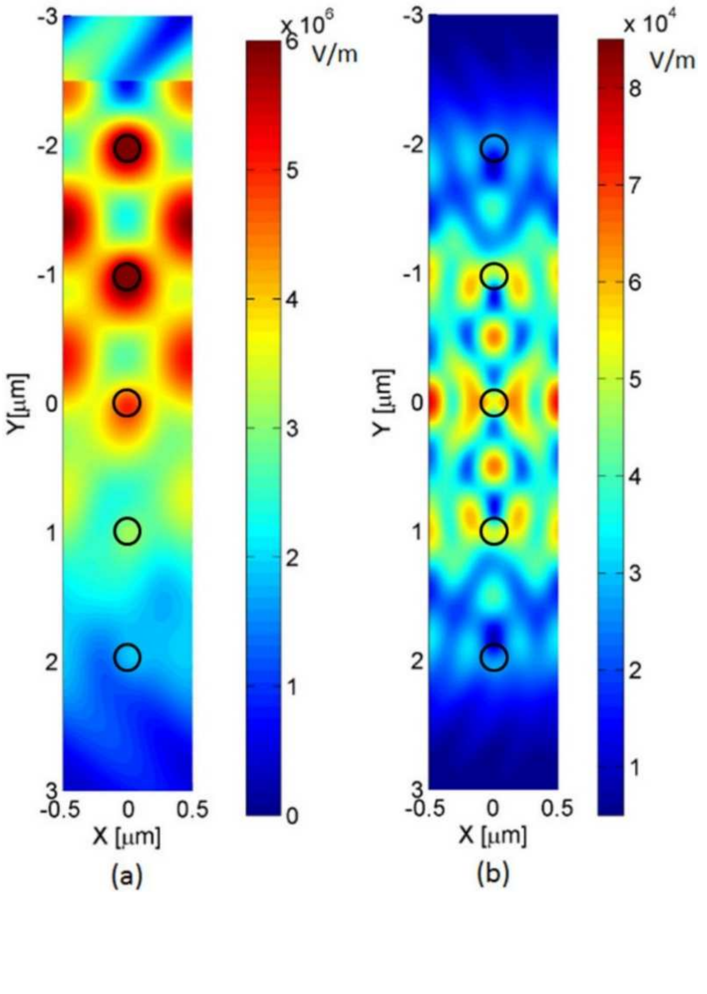

Figure 3. *Magnitude of the E_z field components for*

(a) fundamental wave

(b) second harmonic wave at the resonant frequency for five arrays of cylinders.

We show here the result of a model calculation: the underlying dielectric structure consists of periodic arrays of nonlinear cylinders, it is infinite in the x-direction and there are five periods in the y-direction. The fundamental wave propagates in the positive y-direction, and it can be tilted from normal incidence. At certain angles and frequencies, the structure exhibits double resonance: the reflectivity is close to unity both for the fundamental and for the second harmonic wave.

Grants

NKFIH FK 124723J From topologically protected states to a topological quantum computer (J. Asbóth, 2017-2021)

NKFIH PD 120975 Dynamics of hybrid quantum systems (O. Kálmán, 2016-2019)

NKFIH K 124351 Dynamics and measurement of coherent and open quantumoptical networks (T. Kiss, 2017-2021)

National Excellence Program for Quantum Technology, HunQuTech Consortium: Preparation, distribution of quantum bits and development of quantum information networks (2017-1.2.1-NKP-2017-00001, 2017-2021)

International cooperation

Czech Technical University in Prague (Igor Jex) – Iterative dynamics of quantum systems (T. Kiss)

Technical University, Darmstadt (Gernot Alber) – Dynamics and Control of Quantum Networks (T. Kiss)

University of Osnabrück – Small polarons in luminescent $LiNbO_3$: From bulk crystals to nanocrystals (Z. Kis)

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See also: R-A.6

INSTITUTE FOR PARTICLE AND NUCLEAR PHYSICS*

* **Abbreviations in the researcher lists of the scientific projects:**

#: PhD student

A: associate fellow

E: professor emeritus

R-C. Gravitational physics

Mátyás Vasúth, Dániel Barta#, Károly Zoltán Csukás#, Balázs Kacskovics, István Rácz, László Somlai#

The research projects of the Gravitational Physics Research Group at Wigner RCP are focusing on investigations in theoretical physics related to gravitational phenomena. Our group members have solid background in general relativity and particle physics. As members of the Virgo Scientific Collaboration operating the Virgo detector, the European gravitational wave observatory, the main motivation of our research interest originates from gravitational wave (GW) physics. The scientific results of the last year are summarized below.

Gravitational waves. — The joint 1-month data taking period of the LIGO and Virgo observatories at the second half of 2017 has been concluded with important results. The first three detector observation of a black hole collision was achieved. Moreover, the merger of two neutron stars was also recorded with gravitational waves and electromagnetic observations representing a breakthrough in multi-messenger astronomy. 2018 marks the preparation for the upcoming observation period starting early in 2019. Following the two observation campaigns the time for an extensive upgrade of the observatories has come. As a result of the enhancements an overall 1.5-2 fold increase in sensitivity is expected resulting in an increase in detection rate during the next observation run.

In 2018 the members of our group have participated in the work of the Compact Binary Coalescence (CBC) group with contributions to the description of compact binary sources and their radiation. The accuracy of the software package *CBwaves* developed by our group for the description of the motion and gravitational radiation of compact binary sources was further improved. It was used to study high mass systems and binary evolution in eccentric orbits.

Fast prediction and evaluation of eccentric inspirals using reduced-order models. — A large number of theoretically predicted waveforms are required by matched-filtering searches for the gravitational wave signals produced by compact binary coalescence. In order to substantially alleviate the computational burden in gravitational wave searches and parameter estimation without degrading the signal detectability, we proposed a novel reduced-order-model (ROM) approach with applications to adiabatic 3PN-accurate inspiral waveforms of nonspinning sources that evolve on either highly or slightly eccentric orbits. We provided a singular-value decomposition-based reduced basis method in the frequency domain to generate reduced-order approximations of any gravitational waves with acceptable accuracy and precision within the parameter range of the model (Fig. 1). We constructed efficient reduced bases comprised of a relatively small number of the most relevant waveforms over 3-dimensional parameter space covered by the template bank (total mass $2.15M_\odot \le M \le 215M_\odot$, mass ratio $0.01 \le q \le 1$, and initial orbital eccentricity $0 \le e_0 \le 0.95$). The ROM was designed to predict signals in the frequency band from 10 Hz to 2 kHz for aLIGO and a Virgo design sensitivity. Besides moderating the data reduction, finer sampling of fiducial templates improved the accuracy of surrogates. Considerable increase in the speedup from several hundreds to thousands has been achieved by evaluating surrogates for low-mass systems especially when combined with high-eccentricity (Fig. 2).

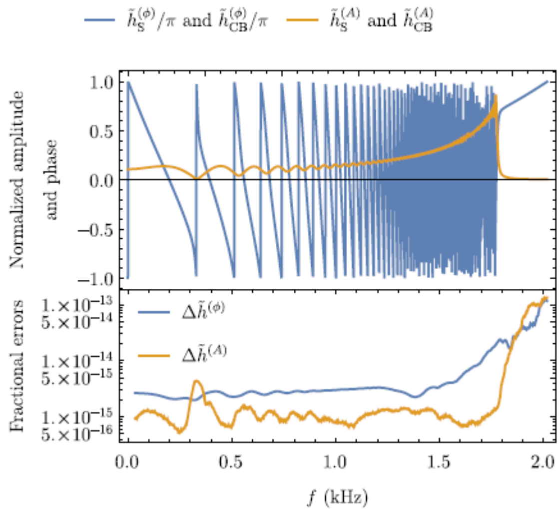

Figure 1. *Top panel: The amplitude and the phase part of the waveform associated with l=1. There is visual agreement among the fiducial* CBwaves *waveform and its surrogate prediction throughout the entire frequency range. Bottom panel: The relative errors with moving average of 50 points in the amplitude and the phase difference between the fiducial waveform and its surrogate model prediction. The differences are smaller than the errors intrinsic to the surrogate model itself, as well as those of state-of-the-art numerical relativity simulations.*

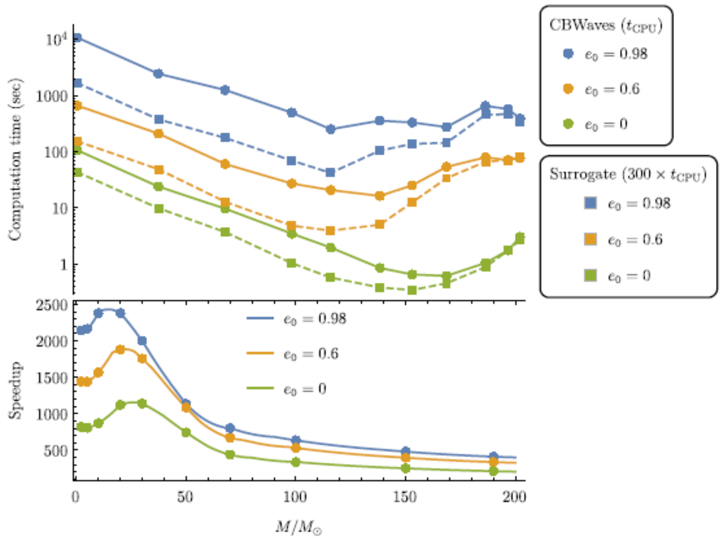

Figure 2. Top panel*: Computational time t_{CPU} to generate fiducial waveforms by CBwaves code (dots; connected by solid lines) against the cost of evaluating corresponding surrogates by ROM (rectangles connected by dashed lines). The computational time was measured for three different initial eccentricities of equal-mass configurations, each associated with different colours.* Bottom panel*: The speedup in evaluating the surrogate model is several thousand times faster around 10-50 $M_\odot$ than generating CBwaves waveforms. For high total mass the speedup falls off to several hundreds. The speedup is roughly twice as great for configurations having extremely high initial eccentricity at $e_0=0.98$ (blue line) as for circular ones at $e_0=0$ (green line)..*

Classical and quantum aspects of canonical gravity. — General relativity is usually formulated in terms of equations for the space-time metric through the Einstein equations. In the canonical formulation of gravity, the field equations are reformulated into a set of constraints and a set of evolution equations to form a constrained Hamiltonian system. These equations then allow for a well-defined initial value problem. In this canonical picture, we have introduced a completely new evolutionary form of the constraint equations in Maxwell theory, in analogy with some recent results on the constraints of general relativity, regardless of the signature and dimension of the ambient space. As an important additional result a new geometric characterization and identification of the Kerr black hole was given in the set of distorted black hole spacetimes.

Mátra Gravitational and Geophysical Laboratory. — The low frequency part of the gravitational wave spectrum below 20 Hz in inaccessible by present ground based observatories. To detect signals in this low frequency band a new infrastructure is planned. The European initiative Einstein Telescope aims to reduce the effect of seismic and Newtonian noises with underground operation, cryogenic facilities and additional technical improvements.

In the Mátra Gravitational and Geophysical Laboratory, we have carried out long-term seismic, infrasound and electromagnetic measurements. In 2018 based on the almost 2 years of data collected so far the members of our group were working on the specification of the quantities for the site selection of 3rd generation underground GW facilities. As a recommendation to the community, we have analyzed and presented different seismic noise measures to use in site characterization. Moreover, with the analyzation of the available long-term measurements we have examined the monthly and yearly variation of seismic noise, which are important local features for e.g. the Einstein Telescope.

Outreach. — To prepare for the next observation period gravitational wave observatories have undergone significant upgrades and changes in 2018 resulting in a 1.5-2 fold increase in their sensitivity. Meanwhile, thoroughly analyzing the data already collected during the previous scientific data taking periods, the collaboration announced four new gravitational wave events not published before. As members of the Virgo Outreach group, we have actively participated in public outreach, the public announcement of data from previous measurements and the first gravitational wave transient catalog containing all the 11 events registered so far. Moreover, several scientific and public lectures were held by our group members for scientists and students. They have actively participated also in the popularization of the European based 3rd generation gravitational wave observatory, the Einstein Telescope.

Grants

OTKA K-115434: Developing and applying new methods to solving the Cauchy problem in general relativity (I. Rácz, 2015-2019)

NKFI K-124366: Geophysical noises in gravitational wave detection (P. Ván, 2017-2020)

Marie Skłodowska-Curie grant No. 665778: Canonical gravity (I. Rácz, 2018-2019)

Short Term Scientific Mission, Theoretical Astrophysics Department, University of Tübingen, Germany, 4th – 20th April 2018. Supported by PHAROS Short Visit Grants, COST Action CA16214 (D. Barta)

EMMI Grant, NTP-NFTÖ-18-B-0390 (D. Barta, 2018)

New National Excellence Program of the Ministry of Human Capacities, Supported BY the ÚNKP-18-3-I (L. Somlai, 2018)

International cooperation

Virgo Scientific Collaboration (M. Vasúth, D. Barta, L. Somlai)

PHAROS COST action CA16214, (Hungarian Representatives: G.G. Barnaföldi, M. Vasúth, 2017-2021)

G2NET COST action CA17137, (Hungarian Representatives: M. Vasúth, M.F. Nagy-Egri, 2018-2022)

CREDO project (L. Somlai)

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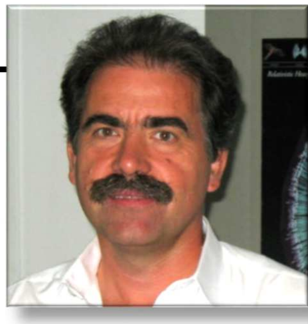
R-D. Femtoscopy



Tamás Csörgő, Gábor Kasza#, Dániel Kincses#, Frigyes Nemes, Tamás Novák, István Szanyi, András Ster

The Femtoscopy Research Group is actively participating both in **theoretical and experimental research**. The **PHENIX** experiment at the RHIC accelerator is in the data analysis phase at Brookhaven National Laboratory publishing in Nature Physics in 2018, while the **TOTEM** experiment at Large Hadron Collider (LHC) at CERN continued its data taking and data analysis as well. During 2018, we have achieved important breakthroughs in theory, as well as in PHENIX and also in TOTEM.

In our **theoretical femtoscopy related research**, related to proton-proton and heavy ion physics at RHIC and LHC,

- We have written a series of four manuscripts on a new family of exact solutions of 1+1 dimensional relativistic fireball hydrodynamics with acceleration and realistic equation of state.
- As applications, we have evaluated the pseudorapidity distributions, the longitudinal HBT radii and the initial energy density in proton-proton and heavy ion collisions at RHIC and LHC.

We have reached a **break-through** in our **theoretical femtoscopy** research related to imaging of the **internal structure of the protons** at LHC energies. With our model-independent Lévy imaging method,

- We have reconstructed the scattering amplitude of high-energy proton-proton elastic scattering processes and determined the excitation function of the shadow profile P(b) of elastic proton-proton and proton-antiproton collisions at the TeV scale.
- **We have identified** significant differences of the four-momentum transfer dependence of the elastic slope B(t) between proton-proton and proton-antiproton collisions, **a clear-cut Odderon effect, indicating the discovery of a new quasi-particle at LHC,** a vector glueball - a quarkless bound state of odd, predominantly 3, number of gluons.

In our **experimental femtoscopy research in the CERN LHC experiment TOTEM**, we have made significant contributions to the

- measurement of the differential cross-section of elastic proton-proton (pp) collisions at 13 TeV
- measurement of the differential cross-section of elastic pp collisions at 2.76 TeV, and to the

- publication of the first measurements of the pp total cross-section at 13 TeV.
- For these achievements, the **Hungarian TOTEM group** received the **2018 TOTEM Achievement Award** and F. Nemes the **2018 TOTEM Publication Award**.

In our **PHENIX related femtoscopy research**, we have made two important discoveries in 2018:

- In p+Au, d+Au and ^{3}He+Au collisions at $\sqrt{s_{NN}}$ = 200 GeV feature **droplets of a perfect fluid with three distinct geometries** on the femtometer scale, thus tiny droplets of strongly interacting quark gluon plasma can be engineered. This PHENIX result was published in **Nature Physics**.
- In 0-30% central Au+Au collision at 200 GeV, the shape of the Bose-Einstein correlation function is significantly different from the Gaussian shape, however, the Levy form describes these data precisely. The PHENIX paper on **Levy stable Bose-Einstein correlations** in $\sqrt{s_{NN}}$ = 200 GeV Au+Au collisions indicated results that are not inconsistent with a **significant mass drop of η' mesons**.

Grants

Hungarian Academy of Sciences - Ukrainian Academy of Science bilateral grant NKM-092/2016 (T. Csörgő)

Hungarian Academy of Sciences - Ukrainian Academy of Science bilateral grant NKM-092/2017-18

Hungarian Academy of Sciences – Grant for the Organization of the BGL 2017 conference

Participation, NKTIH FK 123842 and FK 123959 grants (PI: M. Csanád, ELTE & A. László, Wigner)

Participation in EFOP EFOP 3.6.1-16-2016-00001 grant (PI: Papp József, EKE)

Participation in WG0839/2018 Circles of Knowledge Club – Wigner RCP sponsorship agreement

International cooperations:

PHENIX Collaboration (Brookhaven National Laboratory, USA): Memorandum of Understanding between the PHENIX Experiment and KFKI representing the PHENIX-Hungary team (Hungarian Principal Investigator: M. Csanád (ELTE), participants in 2018: T. Csörgő, G. Kasza, D. Kincses, T. Novák, J. Sziklai.

TOTEM Collaboration (CERN LHC, Svájc). Hungarian Principal Investigator: T. Csörgő, other participants in 2018: T. Csörgő, F. Nemes, I. Szanyi, J. Sziklai.

CERN, Memorandum of Understanding for Collaboration in the Construction of the TOTEM detector and Memorandum of Understanding for the Maintenance and Operation of the TOTEM detector at LHC (Hungarian Principal Investigator T. Csörgő (Wigner RCP and EKE KRC).

During 2017 this membership lead us to participation in the CMS Precision Proton Spectrometer, too.

Bogoliubov Institute for Theoretical Physics (Kiev, Ukraine): bilateral grant NKM-092/2017-18. Hungarian PI: T. Csörgő, Ukrainian PI: D. Anchiskin

Lund University (Lund, Sweden) – Wigner RCP, Memorandum of Understanding on bilateral collaboration (T. Csörgő, A. Ster, with L. Lönnblad , G. Gustafson and R. Pasechnik from Lund).

State University of New York at Stony Brook (Stony Brook, NY, USA) – Wigner RCP, Memorandum of Understanding on bilateral international collaboration (PIs T. Csörgő, R. Lacey (SUNY SB)). Participants in this collaboration: T. Csörgő, D. Kincses.

Radboud University (Nijmegen, The Netherlands) Bilateral international collaboration. Participants during 2018: T. Csörgő, T. Novák as well as W. Metzer (Nijmegen).

Central China Normal University, Wuhan, China: Bilateral international collaboration. Participants during 2018: T. Csörgő, G. Kasza as well as Z.-F. Jiang (Wuhan).

Publications

Articles

1. Csörgő T, Kasza G, Csanád M, Jiang Z: New exact solutions of relativistic hydrodynamics for longitudinally expanding fireballs. ***UNIVERSE*** **4**:6 69/1-21 (2018)
2. Csörgő T, Kasza G: Scaling properties of spectra in new exact solutions of rotating, multi-component fireball hydrodynamics. ***UNIVERSE*** **4**:4 58/1-14 (2018)
3. Jiang ZF, Yang CB, Csanád M, Csörgő T: Accelerating hydrodynamic description of pseudorapidity density and the initial energy density in p plus p, Cu plus Cu, Au plus Au, and Pb plus Pb collisions at energies available at the BNL Relativistic Heavy Ion Collider and the CERN Large Hadron Collider. ***PHYS REV C*** **97**:6 064906/1-9 (2018)

Others

4. Bryslawskyj J, Csörgő T, Csanád M: PHENIX study of the initial state with forward hadron measurements in 200 GeV p(d)+A and ^{3}He+Au collisions. Accessible online https://arxiv.org/abs/1810.03740 4p (2018) (Proc. XXVIIth International Conference on Ultrarelativistic Nucleus-Nucleus Collisions (Quark Matter 2018), Venezia, Italy 13-19 May 2018)
5. Csörgő T, Pasechnik R, Ster A: Odderon and substructures of protons from a model-independent Levy imaging of elastic proton-proton and proton-antiproton collisions. Accessible online https://arxiv.org/abs/1807.02897v2 (2018)

See also: R-B.28

Phenix collaboration

Due to the high number of publications of the large collaboration in which the research group participated in 2018, here we list only a short selection of appearences in journals with the highest impact factor.Wigner-authors: Csörgő T, Novák T, Sziklai J.

1. Aidala C et al. (Phenix Collaboration): Creation of quark–gluon plasma droplets with three distinct geometries. ***NATURE PHYSICS*** **15**: 1-34 (2018)

2. Adare A et al. (PHENIX Collaboration): Pseudorapidity dependence of particle production and elliptic flow in asymmetric nuclear collisions of p+Al, p+Au, d+Au, and He 3 +Au at $\sqrt{s_{NN}}$ = 200 GeV. ***PHYS REV LETT* 121**:22 222301/1-8 (2018)
3. Aidala C et al. (PHENIX Collaboration): Measurements of multiparticle correlations in d+Au collisions at 200, 62.4, 39, and 19.6 GeV and p+Au collisions at 200 GeV and implications for collective behavior. ***PHYS REV LETT* 120**:6 062302/1-8 (2018)
4. Aidala C et al. (PHENIX Collaboration): Nuclear dependence of the transverse-single-spin asymmetry for forward neutron production in polarized p plus A collisions at $\sqrt{s_{NN}}$ = 200 GeV. ***PHYS REV LETT* 120**:2 022001/1-9 (2018)
5. Adare A et al. (PHENIX Collaboration): Cross section and longitudinal single-spin asymmetry A(L) for forward W-+/- -> mu(+/-)nu production in polarized p plus p collisions at $\sqrt{s}$ = 510 GeV. ***PHYS REV D* 98**:3 032007/1-14 (2018)
6. Adare A et al. (PHENIX Collaboration): Measurement of phi-meson production at forward rapidity in p plus p collisions at root s=510 GeV and its energy dependence from root s=200 GeV to 7 TeVMeasurement of phi-meson production at forward rapidity in p plus p collisions at root s=510 GeV and its energy dependence from $\sqrt{s}$ = 200 GeV to 7 TeV. ***PHYS REV D* 98**:9 092006/1-13 (2018)
7. Aidala C et al. (PHENIX Collaboration): Single-spin asymmetry of J/psi production in p plus p, p plus Al, and p plus Au collisions with transversely polarized proton beams at $\sqrt{s_{NN}}$ = 200 GeV. ***PHYS REV D* 98**:1 012006/1-11 (2018)
8. Aidala C et al. (PHENIX Collaboration): Nonperturbative transverse-momentum-dependent effects in dihadron and direct photon-hadron angular correlations in p plus p collisions at $\sqrt{s}$ = 200 GeV. ***PHYS REV D* 98**:7 072004/1-13 (2018)
9. Adare A et al. (PHENIX Collaboration): Measurement of emission-angle anisotropy via long-range angular correlations with high-p_T hadrons in d + Au and p + p collisions at $\sqrt{s_{NN}}$ = 200 GeV. ***PHYS REV C* 98**:1 014912/1-16 (2018)
10. Adare A et al. (PHENIX Collaboration): Lévy-stable two-pion Bose-Einstein correlations in $\sqrt{s_{NN}}$ = 200 GeV Au+Au collisions. ***PHYS REV C* 97**:6 064911/1-22 (2018)
11. Adare A et al.: Measurements of mass-dependent azimuthal anisotropy in central *p* + Au, *d* + $Au, and ^{3}He + Au collisions at $\sqrt{s_{NN}}$ = 200 GeV. ***PHYS REV C* 97**: 064904/1-11 (2018)
12. Adare A et al. (PHENIX Collaboration): Low-momentum direct-photon measurement in Cu + Cu collisions at $\sqrt{s_{NN}}$ = 200 GeV. ***PHYS REV C* 98**:5 054902/1-11 (2018)
13. Aidala C et al. incl. Csörgő T, Kőfaragó M, Novák T, Ster A, Vargyas M, Vértesi R (PHENIX Collaboration): Production of π^0 and η mesons in Cu Ó Au collisions at $\sqrt{s_{NN}}$ = 200 GeV. ***PHYS REV C* 98**: 054903/1-11

TOTEM Collaboration

Wigner-authors: Csanád M, Csörgő T, Nemes F, Novák T, Sziklai J.

Others

1. Antchev G et al. (TOTEM Collaboration): First determination of the ρ parameter at $\sqrt{s}$ = 13 TeV -- probing the existence of a colourless three-gluon bound state (2018) arXiv: https://arxiv.org/abs/1812.04732

2. Antchev G et al. (TOTEM Collaboration): Elastic differential cross-section measurement at $\sqrt{s}$ = 13 TeV by TOTEM (2018). arXiv: https://arxiv.org/abs/1812.08283
3. Antchev G et al. (TOTEM Collaboration): Elastic differential cross-section dσ/dt at $\sqrt{s}$ = 2.76 TeV and implications on the existence of a colourless 3-gluon bound state (2018) arXiv: https://arxiv.org/abs/1812.08610

See also: R-F CMS Collaboration 24

R-F. Hadron physics

Ferenc Siklér, Gyula Bencédi, Zoltán Fodor[A], Endre Futó[A], Sándor Hegyi, Gábor Jancsó[A], József Kecskeméti[A], Gabriella Pálla[E], Zoltán Seres[A], Mónika Varga-Kőfaragó, Róbert Vértesi

The aim of our research group is to better understand the strong interaction through collisions of nucleons and nuclei by performing basic and advanced measurements (cross sections, particle spectra and correlations), and by testing various theoretical ideas (quark-gluon plasma, gluon saturation, critical endpoint of the phase diagram). We participate in several complementary experiments (mainly ALICE and CMS), both in data-taking and physics analysis.

Quantum correlations. — We have finally published a paper on short-range two-particle correlation functions of identified hadrons in pp, p-Pb, and peripheral Pb-Pb collisions at LHC energies. The extracted radii of the particle-emitting source (via Bose-Einstein correlations) are in the range 1-5 fm, reaching highest values for very high multiplicity p-Pb and Pb-Pb collisions (Fig 1, left). The dependence of the radii on the multiplicity and pair transverse momentum factorizes and appears to be less sensitive to the type of the collision system and center-of-mass energy. The observed similarities may point to a common critical hadron density reached in the collisions.

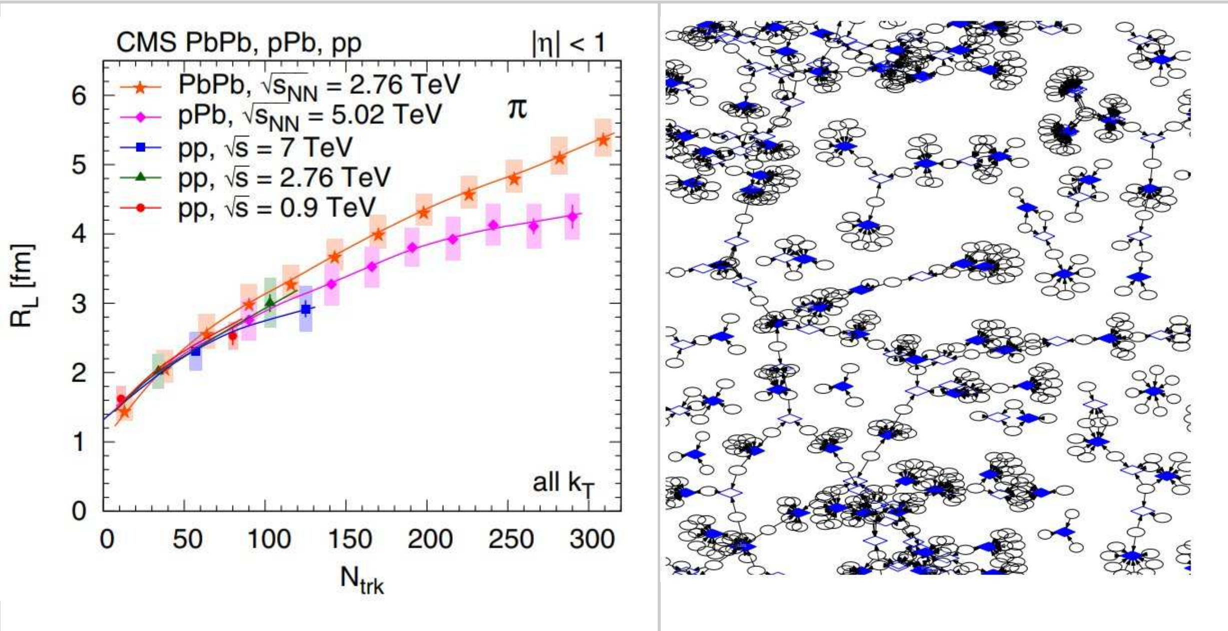


Figure 1. *Left: Track-multiplicity dependence of the two-dimensional pion radius parameters obtained from fits for all collision systems studied. Lines are drawn to guide the eye.. Right: A small fraction of the bipartite graph of hits (ellipses) and track candidates (diamonds) for an event with multiple (40) pp collisions. Directed arrows, graph edges, show potential hit-to-track candidate assignments.*

Novel reconstruction methods. — We have published a paper on a novel combination of established data analysis techniques for the reconstruction of all tracks of primary charged particles created in high-energy collisions. Suitable track candidates are selected by transforming measured hits to a binned track parameter space. Subsequently, their number is further narrowed down by a Kalman filter-based technique. Track candidates and their corresponding hits form a highly connected network, a bipartite graph, where one allows for multiple assignments of hits to track candidates (Fig 1, right). The graph is cut into very many mini-graphs by removing a few of its components. Finally, the hits are distributed among the track candidates by exploring a deterministic decision tree. Simplified models of LHC silicon trackers are employed to study the performance of the proposed method in the case of single or many simultaneous proton-proton collisions, and for single heavy-ion collisions.

In addition, we have developed another track reconstruction method, which uses of both local and global information while keeping competing choices open. The measured hits of adjacent tracking layers are clustered first with help of a mutual nearest neighbor search in angular distance. The resulted chains of connected hits are used as initial clusters for the robust *k*-medians clustering. This latter proceeds by alternating between the hit-to-track assignment and the track-fit update steps, until convergence. The calculation of the hit-to-track distance and that of the track-fit χ2 is performed through the global covariance of the measured hits. The clustering is complemented with elements from a more sophisticated Metropolis-Hastings MCMC algorithm, with the possibility of adding new track hypotheses or removing unnecessary ones.

Angular-correlation measurements. — We have analyzed the Pb-Pb data taken by the ALICE collaboration in 2015, and we have shown new preliminary results from it at The 27th International Conference On Ultrarelativistic Nucleus-Nucleus Collisions (QM 2018) on unidentified two-particle angular correlations in Pb-Pb and pp collisions. The presented new results exhibit a similar broadening of the jet peak towards central collisions at low transverse momentum in Pb-Pb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV as was seen previously at $\sqrt{s_{NN}}$ = 2.76 TeV (Fig 2, left). The results were accepted for publication in Nuclear Physics A. In addition, we are working on the analysis of different Monte Carlo simulations to determine the origin of the observed phenomena. We are analyzing both unidentified and identified two-particle correlations, and the results were presented on a poster at the International Conference on Hard and Electromagnetic Probes of High-Energy Nuclear Collisions in 2018.

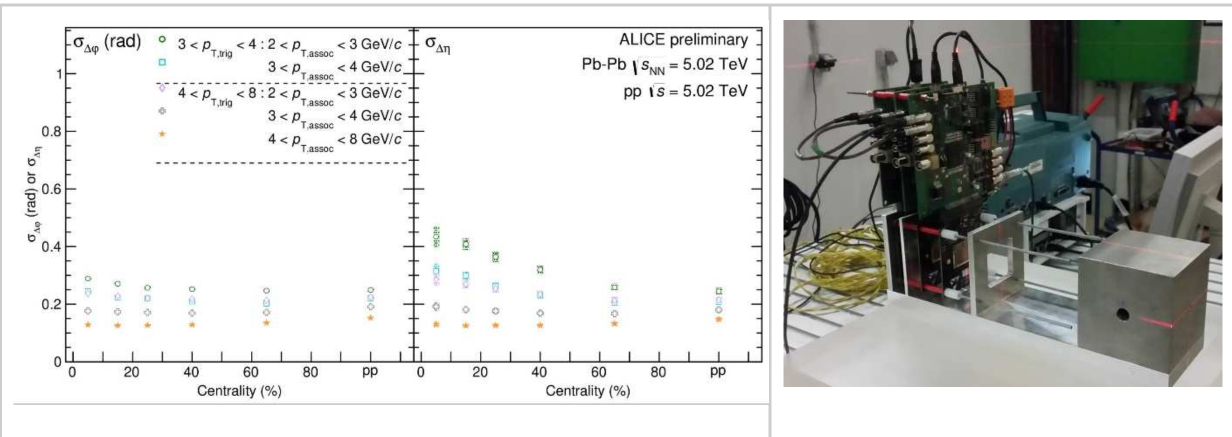


Figure 2. *Left: Width of the jet peak from two-particle angular correlations in Pb-Pb collisions at* $\sqrt{s_{NN}}$ *= 5.02 TeV as a function of centrality. The rightmost points show results from pp collisions at the same energy for comparison. Right: Test beam setup used for the characterization of detectors to be used as a sampling calorimeter for the medical application.*

Medical applications of high-energy detector technologies. — We have joined the development of a sampling calorimeter to be used for imaging in cancer therapy. Cancer tumors can be killed by irradiating them by photons or hadrons. In the case of the treatment by hadrons, the energy deposition and therefore the destructive effect can be focused into the tumor with changing the energy of the hadron beam. In the case of photons, however, most of the energy is deposited at the entrance of the beam. This means that in the treatment with hadrons, the patient receives less unnecessary dose and the treatment can be applied closer to critical organs. However, to reach the full potential of such a treatment the imaging of the patient has to be done by hadrons (mostly commonly protons) as well. We are developing a calorimeter based on the silicon detector developed for the upgrade of the Inner Tracking System of ALICE for such imaging purposes. Our group is taking part in the analysis of the test beam data that will determine whether the chosen detector is suitable for this lower energy regime compared to its original purpose at the LHC(Fig 2, right).

Production of (un)identified particles in pp collisions. — The transverse momentum (p_T) spectra of light-flavor hadrons in pp collisions measured over a broad p_T range provide important input for the study of particle production mechanisms in the soft and hard scattering regime of Quantum Chromodynamics (QCD). We have measured the inclusive, as well as multiplicity-dependent, charged particle transverse momentum distributions for pp collisions at different center-of-mass energies at the ALICE experiment. For pp collisions at $\sqrt{s}$ = 13 TeV and for a fixed multiplicity interval, the parameters obtained from the blast wave analysis of momentum spectra are used to characterize the evolution of the spectral shapes for different event topologies. The multiplicity and spherocity dependencies of the average transverse momenta and integrated yields as a function of charged-particle multiplicity are investigated. The average p_T is larger (smaller) in “jetty” (isotropic) events hinting at different dynamics of particle production. The evolution of the proton-to-pion and kaon-to-pion particle ratios as a function of p_T suggest that the collective-like behavior can be controlled by transverse spherocity. The hadron yields scale with charged-particle multiplicity across different $\sqrt{s}$ and colliding systems, which indicates that hadrochemistry, is dominantly driven by multiplicity. The QCD-inspired models describe several aspects of data. These results were presented at The 27th International Conference on Ultrarelativistic Nucleus-Nucleus Collisions (QM 2018).

Heavy-flavour production. — Heavy-flavour (beauty and charm) quarks are produced almost exclusively in initial hard processes, and their yields remain largely unchanged throughout a heavy-ion reaction. Nevertheless, they interact with the nuclear matter in all the stages of its evolution. Thus, heavy quarks serve as ideal self-generated penetrating probes of the strongly interacting QGP. Jets containing heavy flavour hadrons probe the influence of mass and color-charge effects on fragmentation, as well as provide insight to gluon splitting processes. The ALICE detector has the unique capability of measuring beauty-jets down to relatively low momenta. Our group plays a leading role in ALICE beauty-jet measurement in p-Pb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV (Fig 3, left).

Jet structures. — Collective behavior of high multiplicity events in small systems have also been observed in the heavy-flavour sector. Recent analyses of pp and p-Pb collisions show a universal enhancement of heavy-flavour particles that is usually attributed to multiple parton interactions and higher gluon radiation associated with short distance production processes. We have carried out extensive studies using the PYTHIA8 as well as the HIJING++ Monte-Carlo event generators. We have given predictions for multiplicity-dependent jet structures, and proposed a way to validate the presence and extent of effects such as multiple-parton interactions or color reconnection (Fig 3, right). We have demonstrated that vacuum QCD effects can modify the jet structure, as well as two-particle angular correlation pictures, in high-multiplicity events. We also gave predictions to flavour-dependence of jet shape modification vs. momentum and multiplicity. We have also introduced a definition of a characteristic jet size measure that is independent of multiplicity. We started the experimental analysis of jet shapes in ALICE Run-2 data in cooperation with the CCNU ALICE group in order to verify or exclude the presence of jet-modification by vacuum-QCD effects.

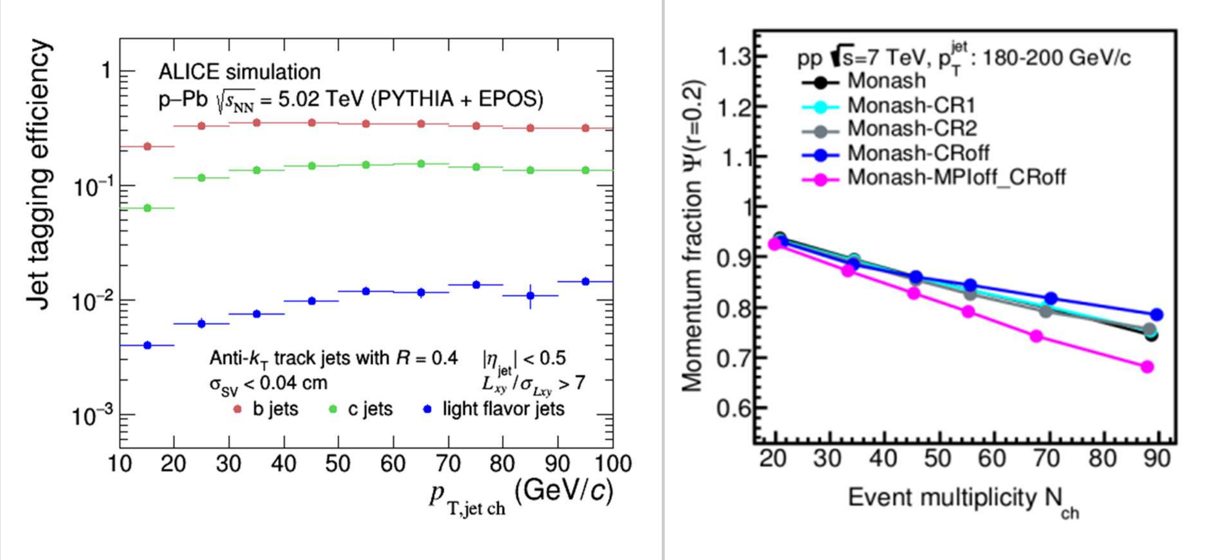


Figure 3. *Left: Tagging efficiencies of beauty, charm and light flavour jets in p-Pb collisions at $\sqrt{s_{NN}}$=5.02 TeV in the ALICE experiment. Right: Modification of the jet structures by multiple-parton interactions and different color reconnection schemes in simulations with PYTHIA8.*

Grants

NKFIH K 128786: Consortional assoc.: Novel tests of the strong interaction with the CERN CMS experiment (F Siklér, 2018-2022)

NKFIH K 120660: Investigation of the identified hadron production in the heavy-ion collisions at the high-luminosity LHC by the ALICE experiment (GG Barnaföldi, 2016-2020)

International cooperation

ALICE, CMS, FOPI, NA49, and NA61 (CERN), PHENIX and STAR (RHIC)

Publications

Articles

1. Münzer R et al. incl. Fodor Z, Kecskeméti J, Seres Z [70 authors]: Determination of N* amplitudes from associated strangeness production in p+p collisions. ***PHYS LETT B* 785**: 574-580 (2018)
2. Siklér F: A combination of analysis techniques for efficient track reconstruction of high multiplicity events in silicon detectors. ***EUR PHYS J A* 54**:6 113/1-11 (2018)

CMS Collaboration

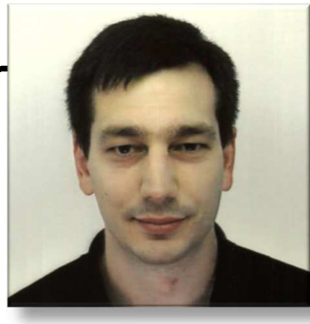
Due to the vast number of publications of the large collaborations in which the research group participated in 2015, here we list only a short selection of appearences in journals with the highest impact factor. Wigner authors in the Collaboration are: Bencze G, Hajdú C, Horváth D, Hunyadi Á, Siklér F, Vámi TÁ, Veszprémi V, Vesztergombi G, Zsigmond AJ.

1. Sirunyan AM et al. (CMS Collaboration) [2289 authors]: Elliptic flow of charm and strange hadrons in high-multiplicity *p*+Pb collisions at $\sqrt{s_{NN}}$ = 8.16 TeV. ***PHYS REV LETT*** **121**:8 082301/1-18 (2018)
2. Sirunyan AM et al. (CMS Collaboration) [2300 authors]: Observation of the χ_{b1}(3P) and χ_{b2}(3P) and measurement of their masses. ***PHYS REV LETT*** **121**:9 092002/1-17 (2018)
3. Sirunyan AM et al. (CMS Collaboration) [2228 authors]: Constraining gluon distributions in nuclei using dijets in proton-proton and proton-lead collisions at $\sqrt{s_{NN}}$ = 5.02 TeV. ***PHYS REV LETT*** **121**:6 62002/1-18 (2018)
4. Sirunyan AM et al. (CMS Collaboration) [2239 authors]: Measurement of prompt D^0 meson azimuthal anisotropy in Pb-Pb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV. ***PHYS REV LETT*** **120**:20 202301-1-17 (2018)
5. Sirunyan AM et al. (CMS Collaboration) [2259 authors]: Search for the X (5568) State Decaying into $B_s^0\pi^{\pm}$ Bs0 π± in proton-proton collisions at $\sqrt{s}$ = 8 TeV. ***PHYS REV LETT*** **120**:20 202005/1-17 (2018)
6. Sirunyan AM et al. (CMS Collaboration) [2290 authors]: Search for heavy neutral leptons in events with three charged leptons in proton-proton collisions at $\sqrt{s}$ = 13 TeV. ***PHYS REV LETT*** **120**:22 221801/1-20 (2018)
7. Sirunyan AM et al. (CMS Collaboration) [2301 authors]: Search for narrow resonances in the *b*-tagged dijet mass spectrum in proton-proton collisions at $\sqrt{s}$ = 8 TeV. ***PHYS REV LETT*** **120**:20 201801/1-19 (2018)
8. Sirunyan AM et al. (CMS Collaboration) [2229 authors]: Suppression of excited Υ states relative to the ground state in Pb-Pb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV. ***PHYS REV LETT*** **120**:14 142301/1-17 (2018)
9. Sirunyan AM et al. (CMS Collaboration) [2258 authors]: Measurement of the splitting function in *pp* and Pb-Pb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV. ***PHYS REV LETT*** **120**:14 142302/1-17 (2018)
10. Sirunyan AM et al. (CMS Collaboration) [2301 authors]: Observation of $t\overline{t}H$ production. ***PHYS REV LETT*** **120**:23 231801/1-17 (2018)
11. Sirunyan AM et al. (CMS Collaboration) [2290 authors]: Search for physics beyond the standard model in events with high-momentum Higgs bosons and missing transverse momentum in proton-proton collisions at 13 TeV. ***PHYS REV LETT*** **120**:24 241801/1-17 (2018)
12. Sirunyan AM et al. (CMS Collaboration) [2228 authors]: Observation of correlated azimuthal anisotropy Fourier harmonics in *pp* and *p* + Pb collisions at the LHC. ***PHYS REV LETT*** **120**:9 092301/1-17 (2018)
13. Sirunyan AM et al. (CMS Collaboration) [2265 authors]: Observation of electroweak production of same-sign W boson pairs in the two jet and two same-sign lepton final state in proton-proton collisions at $\sqrt{s}$ = 13 TeV. ***PHYS REV LETT*** **120**:8 081801/1-17 (2018)

14. Sirunyan AM et al. (CMS Collaboration) [2263 authors]: Inclusive search for a highly boosted Higgs boson decaying to a bottom quark-antiquark pair. ***PHYS REV LETT*** **120**:7 071802/1-18 (2018)
15. Sirunyan AM et al. (CMS Collaboration) [2283 authors]: Observation of medium-induced modifications of jet fragmentation in Pb-Pb collisions at $\sqrt{s_{NN}}$ = 5.02 TeV using isolated photon-tagged jets. ***PHYS REV LETT*** **121**:24 242301/1-18 (2018)
16. Sirunyan AM et al. (CMS Collaboration) [2303 authors]: Search for leptoquarks coupled to third-generation quarks in proton-proton collisions at $\sqrt{s}$ = 13 TeV. ***PHYS REV LETT*** **121**:24 241802/1-19 (2018)
17. Sirunyan AM et al. (CMS Collaboration) [2285 authors]: Observation of Higgs boson decay to bottom quarks. ***PHYS REV LETT*** **121**:12 121801/1-20 (2018)
18. Sirunyan AM et al. (CMS Collaboration) [2305 authors]: Evidence for the associated production of a single top quark and a photon in proton-proton collisions at $\sqrt{s}$ = 13 TeV. ***PHYS REV LETT*** **121**:22 221802/1-18 (2018)
19. Sirunyan AM et al. (CMS Collaboration) [2291 authors]: Search for vector-like T and B quark pairs in final states with leptons at $\sqrt{s}$ = 13 TeV. ***J HIGH ENERGY PHYS*** **2018**:8 177/1-51 (2018)
20. Sirunyan AM et al. (CMS Collaboration) [2305 authors]: Search for additional neutral MSSM Higgs bosons in the tau tau final state in proton-proton collisions at $\sqrt{s}$ = 13 TeV. ***J HIGH ENERGY PHYS*** **2018**:9 007/1-60 (2018)
21. Sirunyan AM et al. (CMS Collaboration) [2304 authors]: Search for resonant pair production of Higgs bosons decaying to bottom quark-antiquark pairs in proton-proton collisions at 13 TeV. ***J HIGH ENERGY PHYS*** **2018**:8 152/1-38 (2018)
22. Sirunyan AM et al. (CMS Collaboration) [2290 authors]: Search for disappearing tracks as a signature of new long-lived particles in proton-proton collisions at $\sqrt{s}$ = 13 TeV. ***J HIGH ENERGY PHYS*** **2018**:8 016/1-40 (2018)
23. Sirunyan AM et al. (CMS Collaboration) [2258 authors]: Measurement of the cross section for top quark pair production in association with a W or Z boson in proton-proton collisions at $\sqrt{s}$ = 13 TeV. ***J HIGH ENERGY PHYS*** **2018**:8 011/1-50 (2018)
24. Sirunyan AM et al. (CMS and TOTEM Collaborations) [2382 authors]: Observation of proton-tagged, central (semi)exclusive production of high-mass lepton pairs in pp collisions at 13 TeV with the CMS-TOTEM precision proton spectrometer. ***J HIGH ENERGY PHYS*** **2018**:7 153/1-45 (2018)
25. Sirunyan, AM et al. (CMS Collaboration) [2282 authors]: Measurement of the inelastic proton-proton cross section at $\sqrt{s}$ = 13 TeV. ***J HIGH ENERGY PHYS*** **2018**:7 161/1-33 (2018)

See also: R-B: ALICE Collaboration (Varga-Kőfaragó M), R-D PHENIX Collaboration 13

R-H. Standard model and new physics



Viktor Veszprémi, Dániel Barna[A], Tamás Balázs, Lajos Diósi, Csaba Hajdu, Dezső Horváth[E], Martin Novák[#], József Tóth, Tamás Vámi[#], István Wágner[A]

Physics analyses and theoretical work. — The group has contributed to bringing an inclusive search for supersymmetry with boosted objects to publication stage using proton-proton collision data that corresponded to an integrated luminosity of 35.9 fb^{-1}, taken prior to 2017. Exclusion limits on the gluino mass were extended to 2 TeV, while on the stop quark mass to 1.14 TeV. Profiting from the opportunity that the LHC has gone into a more than two-year long shutdown, we have started to reprocess the data we took with the new pixel detector in the last two years using improved calibration and detector description models for further analysis in order to approximately double the analysis sensitivity. We provided a member for the Publication Committee of the CMS Experiment at CERN and played an important role in publishing CMS results of low-x Quantum Chromodynamics (QCD) studies. We hold leadership positions, a group convenor and a deputy project manager, in the CMS Tracker project.

The stable operation of the T2_HU_Budapest grid site continued in 2018. Our site is used extensively by the entire CMS collaboration including our group for reconstructing collision data in physics analyses. The disk capacity committed to CMS has increased to 1 PB.

We proposed a general concept of bosonic operator orderings and generalized Wick's theorem transforming any ordering into any other one. We pointed out how Planckian scale challenges the validity of the massive body Schrödinger equation.

Work on instrumentation. – The group created a test setup for developing the CMS Phase 2 Upgrade Inner Tracker data-acquisition system, and started to develop firmware in order to calibrate and read out the new sensors that are being designed for the upgraded detector. We have constructed a test-beam telescope to be used for the high rate tests of the new Phase 2 Tracker chips; commissioned the telescope and took the first data using the Phase 2 Outer Tracker chip prototypes at the Super Proton Synchrotron (SPS) at CERN.

The SPS Diffuser designed and constructed by our group was successfully installed and tested in the CERN SPS accelerator, and delivered the expected performance in terms of loss reduction. The conceptual design of a high-field extraction septum magnet for the Future Circular Collider was completed, which uses the combination of a superconducting magnet and a passive superconducting shield.

Outreach. – An education program was organized by Wigner RCP at CERN with the leadership of our group: the annual Hungarian Teachers Programme (18-25 August 2018) for 21 physics teachers. For the teachers we organized a meeting on December 8 at Wigner RCP with the lecturers. We also participated in the organization of the annual Hands-on Particle Physics Master-classes on two occasions with 22 high-school students attending each session. We have also participated in the organization of two scientific seminars on particle physics for the

Celebration of Hungarian Science on particle physics at the Hungarian Academy of Sciences and at the Roland Eötvös University. In addition to conference talks and university teaching, many popular lectures were given by our group.

Grants

NKFIH K-124850 Consortional assoc.: The Standard Model and beyond: Searching for New Physics with the CERN LHC CMS experiment (V. Veszprémi, Cs. Hajdu, D. Horváth, T. Vámi, 2017-2021)

NKFIH K-124945 Research and development of novel technologies for particle accelerators (D. Barna, 2017-2021)

Pallas Athene Foundations HTP-2018 (D. Horváth)

FQXi-MGA-1707 Gravity related modifications of non-relativistic quantum theory (L. Diósi, 2017)

International cooperation

CMS Collaboration (over 200 institutes)

University of Tokyo, Japan

RIKEN, Wako, Japan

Max-Planck-Institut für Quantenoptik, Germany

Università di Brescia & Istituto Nazionale di Fisica Nucleare, Italy

Publications

Articles

1. Diósi L: Wick theorem for all orderings of canonical operators. ***J PHYS A-MATH THEOR*** **51**:36 365201/1-6 (2018)
2. Diósi L: Fundamental irreversibility: Planckian or Schrödinger-Newton? ***ENTROPY*** **20**:7 1-5 (2018)
3. Giunchi G, Barna D, Bajas H, Brunner K, Nemet A, Petrone C: Relaxation phenomena in a long MgB_2 tube subjected to transverse magnetic field, at 4.2 K. **IEEE T APPL SUPERCON 28**:4 1-5 (2018)

Others

4. Horváth D: Új felfedezések a CERN Nagy Hadronütköztetőjénél: furcsa részecskék (New inventions at the LHC of CERN: strange particles, in Hungarian). ***FIZIKAI SZEMLE*** **68**:7-8 219-224 (2018)
5. Horváth D, Trócsányi Z: Müon: mi az és mire jó? (Muon: what is it and what good is it?, in Hungarian) ***FIZIKAI SZEMLE*** **68**:5 147-153 (2018)
6. Horváth D: Magyar tanárok és diákok részecskefizikai oktatása a Cern-ben (Hungarian teachers and students learn particle physics at CERN, in Hungarian). ***FIZIKAI SZEMLE*** **68**:4 124-130 (2018)

ATLAS collaboration

Due to the vast number of publications of the large collaborations in which the research group participated in 2018, here we list only a short selection of appearances in journals with the highest impact factor. Wigner author in the collaboration is József Tóth.

1. Aaboud M et al. (ATLAS Collaboration) [2892 authors]: Search for low-mass dijet resonances using trigger-level jets with the ATLAS detector in pp collisions at $\sqrt{s}$ = 13 TeV. ***PHYS REV LETT*** **121**:8 081801/1-20 (2018)
2. Aaboud M et al. (ATLAS Collaboration) [2886 authors]: Measurement of the soft-drop jet mass in *pp* collisions at $\sqrt{s}$ = 13 TeV with the ATLAS detector. ***PHYS REV LETT*** **121**:9 092001/1-21 (2018)
3. Aaboud M et al. (ATLAS Collaboration) [2870 authors]: Search for the decay of the Higgs boson to charm quarks with the ATLAS experiment. ***PHYS REV LETT*** **120**:21 211802/1-20 (2018)
4. Aaboud M et al. (ATLAS Collaboration) [2887 authors]: Search for a structure in the $B_s^0\pi^{\pm}$ invariant mass spectrum with the ATLAS experiment. ***PHYS REV LETT*** **120**:20 202007/1-19 (2018)
5. Aaboud M et al. (ATLAS Collaboration) [authors]: Search for high-mass resonances decaying to $\tau\nu$ in *pp* collisions at $\sqrt{s}$ = 13 TeV with the ATLAS detector. ***PHYS REV LETT*** **120**:16 161802/1-20 (2018)
6. Aaboud M. et al. (ATLAS Collaboration) [2929 authors]: Combination of the searches for pair-produced vectorlike partners of the third-generation quarks at $\sqrt{s}$ = 13 TeV with the ATLAS detector. ***PHYS REV LETT*** **121**:21 211801/1-20 (2018)
7. Aaboud M. et al. (ATLAS Collaboration) [2924 authors]: Search for resonant and nonresonant Higgs boson pair production in the $b\bar{b}\tau^+\tau^-$ decay channel in *pp* collisions at $\sqrt{s}$ = 13 TeV with the ATLAS detector. ***PHYS REV LETT*** **121**:19 191801/1-24 (2018)
8. Aaboud et al. (ATLAS Collaboration) [2900 authors]: Search for supersymmetry in final states with charm jets and missing transverse momentum in 13 TeV *pp* collisions with the ATLAS detector. ***J HIGH ENERGY PHYS*** **2018**:9 050/1-44 (2018)
9. Aaboud M et al. (ATLAS Collaboration) [2913 authors]: Measurements of b-jet tagging efficiency with the ATLAS detector using $t\bar{t}$ events at $\sqrt{s}$ = 13 TeV. ***J HIGH ENERGY PHYS*** **2018**:8 089/1-47 (2018)
10. Aaboud M et al. (ATLAS Collaboration) [2869 authors]: Search for flavour-changing neutral current top-quark decays t → qZ in proton-proton collisions at $\sqrt{s}$ = 13 TeV with the ATLAS detector. ***J HIGH ENERGY PHYS*** **2018**:7 176/1-41 (2018)
11. Aaboud M et al. (ATLAS Collaboration) [2870 authors]: Search for pair production of heavy vector-like quarks decaying into high-p_T W bosons and top quarks in the lepton-plus-jets final state in pp collisions at $\sqrt{s}$ = 13 TeV with the ATLAS detector. ***J HIGH ENERGY PHYS*** **2018**:8 048/1-41 (2018)
12. Aaboud M et al. (ATLAS Collaboration) [2903 authors]: Search for exclusive Higgs and Z boson decays to $\phi\gamma$ and $\rho\gamma$ with the ATLAS detector. ***J HIGH ENERGY PHYS*** **2018**:7 127/1-37 (2018)
13. Aaboud M et al. (ATLAS Collaboration) [2902 authors]: Search for pair production of up-type vector-like quarks and for four-top-quark events in final states with multiple *b*-jets with the ATLAS detector. ***J HIGH ENERGY PHYS*** **2018**:7 089/1-68 (2018)

14. Aaboud M et al. (ATLAS Collaboration) [2900 authors]: Search for Higgs boson decays to beyond-the-Standard-Model light bosons in four-lepton events with the ATLAS detector at $\sqrt{s}$ = 13 TeV. ***J HIGH ENERGY PHYS*** **2018**:6 166/1-51 (2018)
15. Aaboud M et al. (ATLAS Collaboration) [2885 authors]: Search for top-squark pair production in final states with one lepton, jets, and missing transverse momentum using 36 fb^{-1} of $\sqrt{s}$ = 13 TeV *pp* collision data with the ATLAS detector. ***J HIGH ENERGY PHYS*** **2018**:6 108/1-96 (2018)
16. Aaboud M et al. (ATLAS Collaboration) [2874 authors]: Search for supersymmetry in final states with missing transverse momentum and multiple b-jets in proton-proton collisions at $\sqrt{s}$ = 13 TeV with the ATLAS detector. ***J HIGH ENERGY PHYS*** **2018**:6 107/1-58 (2018)
17. Aaboud M et al. (ATLAS Collaboration) [2874 authors]: Search for long-lived charginos based on a disappearing-track signature in *pp* collisions at $\sqrt{s}$ = 13 TeV with the ATLAS detector. ***J HIGH ENERGY PHYS*** **2018**:6 022/1-48 (2018)
18. Aaboud M et al. (ATLAS Collaboration) [2903 authors]: Measurement of inclusive jet and dijet cross-sections in proton-proton collisions at $\sqrt{s}$ = 13 TeV with the ATLAS detector. ***J HIGH ENERGY PHYS*** **2018**:5 195/1-47 (2018)
19. Aaboud M et al. (ATLAS Collaboration) [2880 authors]: Measurement of differential cross sections and W^+/W^- cross-section ratios for *W* boson production in association with jets at $\sqrt{s}$ = 8 TeV with the ATLAS detector. ***J HIGH ENERGY PHYS*** **2018**:5 077/1-60 (2018)
20. Aaboud M et al. (ATLAS and CMS Collaborations) [5098authors]: Combination of inclusive and differential $t\bar{t}$ charge asymmetry measurements using ATLAS and CMS data at $\sqrt{s}$ = 7 and 8 TeV. ***J HIGH ENERGY PHYS*** **2018**:4 033/1-68 (2018)
21. Aaboud M et al. (ATLAS Collaboration) [2907 authors]: Search for heavy resonances decaying into a *W* or *Z* boson and a Higgs boson in final states with leptons and *b*-jets in 36 fb^{-1} of $\sqrt{s}$ = 13 TeV pp collisions with the ATLAS detector. ***J HIGH ENERGY PHYS*** **2018**:3 174/1-53 (2018)
22. Aaboud M et al. (ATLAS Collaboration) [2906 authors]: Measurement of the Higgs boson coupling properties in the $H \to ZZ^* \to 4\ell$ decay channel at $\sqrt{s}$ = 13 TeV with the ATLAS detector. ***J HIGH ENERGY PHYS*** **2018**:3 095/1-60 (2018)
23. Aaboud M et al. (ATLAS Collaboration) [2904 authors]: Search for W W/W Z resonance production in $\ell\nu qq$ final states in pp collisions at $\sqrt{s}$ = 13 TeV with the ATLAS detector. ***J HIGH ENERGY PHYS*** **2018**:3 042/1-45 (2018)
24. Aaboud M et al. (ATLAS Collaboration) [2893 authors]: Searches for heavy ZZ and ZW resonances in the $\ell\ell qq$ and $\nu\nu qq$ final states in pp collisions at $\sqrt{s}$ = 13 TeV with the ATLAS detector. ***J HIGH ENERGY PHYS*** **2018**:3 009/1-53 (2018)
25. Aaboud M et al. (ATLAS Collaboration) [2904 authors]: Search for dark matter and other new phenomena in events with an energetic jet and large missing transverse momentum using the ATLAS detector. ***J HIGH ENERGY PHYS*** **2018**:1 126/1-53 (2018)

See also: R-F CMS Collaboration (Hajdú C, Horváth D, Vámi T)

R-K. Ion beam physics

Edit Szilágyi, István Bányász, Pál Kostka[A], Endre Kótai[A], Imre Kovács, Attila Németh, Zoltán Szőkefalvi-Nagy[E]

Charge accumulation — Insulator materials have scientific and technological importance in diverse areas such as thermo-isolating coatings for spacecraft, optoelectronics solar panels, and applications of polymers, etc. During the bombardment of insulator materials with energetic particles, i.e., during ion implantation or ion beam analysis, the samples are often emitting light and are sparking.

Analysing insulator samples, due to charge accumulation on the beam spot a potential difference ΔU will be formed between the sample surface and the ground (e.g., sample holder), which is able to decelerate the incoming beam particles before they reach the sample and to accelerate the reaction products when they leave the sample surface. These deceleration and acceleration processes will modify the energy spectrum of the reaction products. In addition, due to the sparking, the potential difference ΔU is not stable during the experiments. The fluctuation δU will introduce new energy spread contributions to the conventional ones.

Despite all the efforts to eliminate the charge accumulation using thin cover layers, wrapping or masking the samples, applying relatively low beam currents or electron sources, sometimes the samples may be charged. Ion beam analysis spectrum evaluation code, DEPTH was extended by a module implementing a new model accounting for charging-up effects. The results are shown in Fig.1.

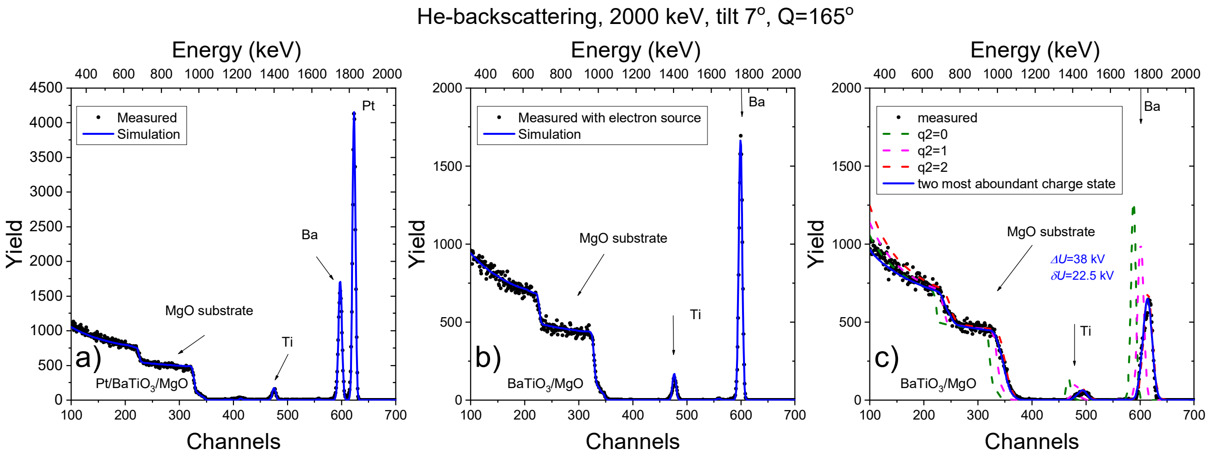
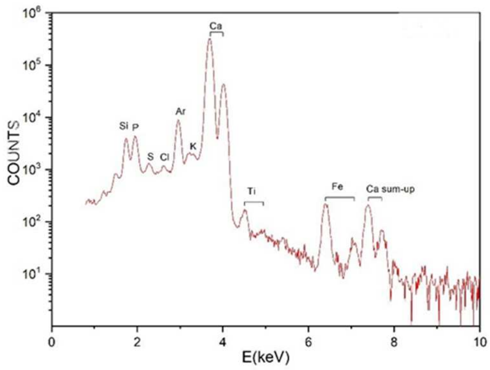


Figure 1. *Comparison of He-BS spectra taken on 30 nm* $BaTiO_3$ *layer on MgO substrate. a) Using Pt cover layer, b) with and c) without electron source. Vertical arrows represent the surface positions of Pt, Ba and Ti according to the energy calibration. Lines for various simulation by DEPTH. In Fig. a) and b) no charge accumulation is occurred. In Fig. c, the sample is charged up to* ΔU*=38 kV,* δU*=22.5kV. Dashed lines represent the charge state of outgoing ions (0, 1 and 2). Solid line represents DEPTH simulation, when the energy dependent charge state distribution is substituted by the two most abundant charge states.*

In Fig 1 2 MeV He-BS spectra taken on $BaTiO_3$ thin layer on MgO substrate are shown. By covering partially the sample with 5 nm thick Pt layer (Fig. 1a) no charge accumulation occurred on the covered region. To eliminate the charge accumulation in the non-covered region, an electron source was used during the experiment (Fig. 1b) while spectra taken without using electron source are shown in Fig. 1c. Due to the energy dependence of the charge distributions, the charging-up spectrum cannot be interpreted by a simply linear combination of simulations calculated for charge states 0, 1 and 2. This is well visible in Fig. 1c. For the correct interpretation of the electrostatically charged up spectrum the energy dependent charge state distribution is substituted with the two most abundant charge states calculated from Z_{mean}, gives a very good agreement with the experiment.

Advanced cultural heritage research. — Archaeological artefacts, blackish grey beads of unknown nature that come from a funerary feature used for the secondary deposition of cremated remains located in the centre of Perdigões (Évora, Portugal) dated from the third quarter of the 3rd millennium BC were studied. In the context of IPERION CH cooperation a wide range of non-destructive techniques were applied, external milli-beam particle induced X-ray emission spectroscopy (PIXE), prompt-gamma activation analysis (PGAA), and high-resolution time-of-flight diffractometer (ToF-ND). In some cases infrared spectroscopic (FTIR) and Scanning Electron Microscopy coupled with Energy Dispersive X-ray Spectrometry (SEM/EDX) measurements were also performed. The surface chemical composition obtained by PIXE and the bulk analysis by PGAA and ToF-ND indicate, that the most probable raw materials for the blackish grey beads manufacture were shells.



The PIXE measurements were performed at the 5MV Van de Graaff accelerator of the Institute of Particle and Nuclear Physics, Wigner Research Centre for Physics, Hungarian Academy of Sciences.

Grants

OTKA K-115852: Development and optical monitoring of nanostructures for sensing (Principal investigator: P. Petrik, HAS Centre for Energy Research, 2015-2018)

EC H2020 Grant No. 654028: Integrated Platform for the European Research Infrastructure on Culture Heritage (IPERION CH, 2015-2019)

European Research Infrastructure for Heritage Science Preparatory Phase, Grant No. 739503 (E-RIHS PP, 2017-2019)

MTA Infrastructure Development: Running costs of some infrastructures of the department of Materials Science by Nuclear methods. (E. Szilágyi 2018)

International cooperation

Nuclear Physics Institute (Řež, Czech Republic, I. Bányász)

Instituto di Fisica Applicata "Nello Carrara" (Sesto Fiorentino, Italy, I. Bányász)

University of Lanzhou (Lanzhou, China, E. Szilágyi)

Campus Tecnológico E Nuclear, Instituto Superior Técnico, Universidade de Lisboa (Lisbon, Portugal, I. Kovács, Z. Szőkefalvi-Nagy)

National Institute for Nuclear Physics and Engineering Horia Hulubei (Bucharest, Romania, I. Kovács, Z. Szőkefalvi-Nagy)

Mureș County Museum (Targu Mures, Romania, I. Kovács, Z. Szőkefalvi-Nagy)

Publications

Articles

1. Constantinescu B, Cristea-Stan D, Szőkefalvi-Nagy Z, Kovács I, Harsányi I, Kasztovszky Zs: PIXE and PGAA – Complementary methods for studies on ancient glass artefacts (from Byzantine, late medieval to modern Murano glass). ***NUCL INSTRUM METH B*** **417**: 105-109 (2018)
2. Dias MI, Kasztovszky Z, Prudêncio MI, Harsányi I, Kovács I, Szőkefalvi-Nagy Z, Mihály J, Káli G, Valera AC, Rodrigues AL: Investigating beads from Chalcolithic funerary cremation contexts of Perdigões, Portugal. ***J ARCHAEOL SCI REP*** **20**: 434-442 (2018)
3. Dias MI, Kasztovszky Zs, Prudêncio MI, Valera AC, Maróti B, Harsányi I, Kovács I, Szőkefalvi-Nagy Z: X-ray and neutron-based non-invasive analysis of prehistoric stone artefacts: a contribution to understand mobility and interaction networks. ***ARCHAEOL ANTHROP SCI*** **10**:6 1359-1373 (2018)
4. Zolnai Zs, Zámbó D, Osváth Z, Nagy N, Fried M, Németh A, Pothorszky Sz, Szekrényes DP, Deák A: Gold nanorod plasmon resonance damping effects on a nanopatterned substrate. ***J PHYS CHEM C*** **122**:43 24941-24948 (2018)

Conference proceedings

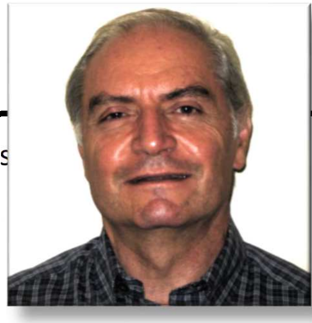
5. Bányász I, Pelli S, Nunzi-Conti G, Righini GC, Berneschi S, Szilágyi E, Németh A, Fried M, Petrik P, Agócs E, Kalas B, Zolnai Z, Khanh NQ, Rajta I, Nagy GUL, Havranek V, Vosecek V, Veres M, Himics L: Design, Ion beam fabrication and test of integrated optical elements. In: *Proc 6th International Conference on Photonics, Optics and Laser Technology (PHOTOPTICS 2018), Funchal, Madeira – Portugal, 25-27 January, 2018.* Eds: Raposo M, Ribeiro PA, SciTePress, (2018) pp. 279-285

See also: R-P W7X Collaboration (Szőkefalvi-Nagy Z)

Dinklage et al. Erratum to: Magnetic configuration effects on the Wendelstein 7-X stellarator (Nature Physics, (2018), 14, 8, (855-860), 10.1038/s41567-018-0141-9)

Pisano, F. et al. Towards a new image processing system at Wendelstein 7-X: From spatial calibration to characterization of thermal events

R-L. Cold plasma and atomic physics in strong fields



Gagik Dzsotjan, József Bakos, Gábor Demeter, Dávid Dzsotjan, Miklós
Zsuzsanna Sörlei[A]

Time-resolved diagnostics of rubidium laser plasma column in longitudinal direction. — Successful acceleration of electrons in AWAKE (advanced wake field acceleration) experiment at CERN in 2018, [1] was an important milestone in developing of new alternative ways of particle acceleration to high-energy domain. The main goal of the AWAKE experiment is to show possibilities to accelerate electrons (positrons) to TeV energies in a single acceleration stage by utilizing the proton bunch available at Large Hadrons Collider. An extended volume of extremely homogeneous plasma is an indispensable part of the acceleration scheme. This plasma is used for splitting the LHC proton bunch into micro-bunches using self-modulation instability in the plasma to provide coherent wake-field acceleration of electrons by the proton bunch. Determination of parameters of the plasma column created by ionization of the medium (rubidium vapor) by strong ultra-short laser pulses is extremely important for efficient wake-field acceleration of the particles in the plasma.

Our research was focused on characterization of the plasma channel induced in a cell with Rb vapor through ionizing the Rb atoms by ultra-short laser pulses. The experiments were conducted in our “clean room” lab with a Ti:Sa laser system Hydra of Coherent Co. with pulse energy about 25-30 mJ and pulse duration of 30-40 fs.

We used interferometric scheme for characterization of the plasma channel similar to our previous scheme (Fig.1). The measurements were performed by a CW diode laser with frequency close to D2 line of Rb.

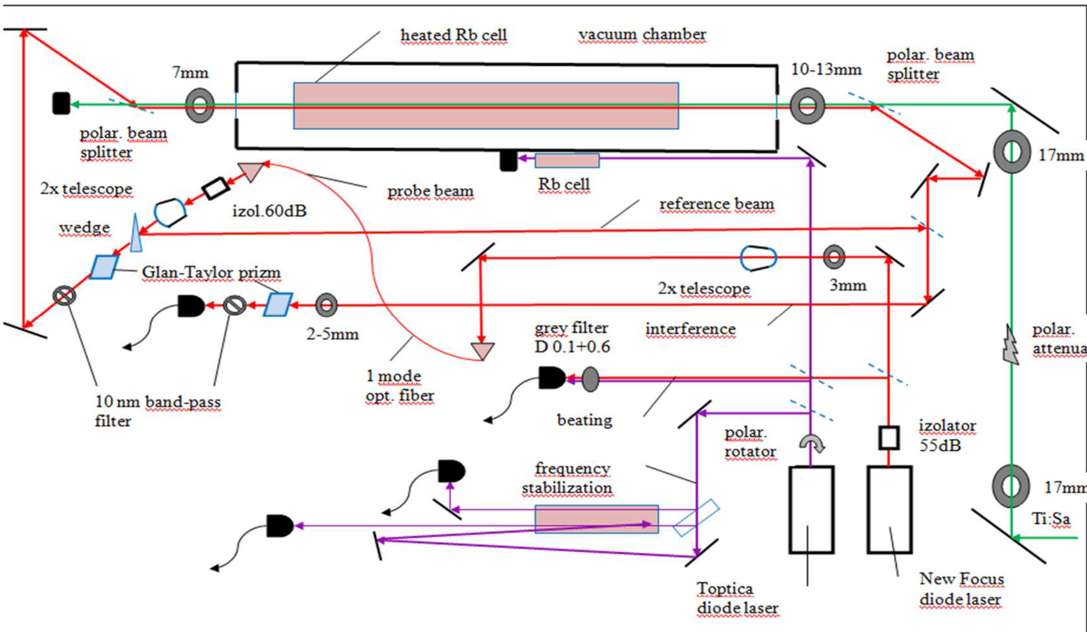


Fig.1. The scheme of the real-time interferometric diagnostic scheme.

Accordingly, the probe diode laser beam propagates in direction opposite to the ionizing laser pulse through a glass cell filled with Rb vapor located in one arm of the interferometer. This probe beam creates a fringe pattern with a reference beam from the same laser propagating in the air in the other arm of the interferometer.

Time variation of the interferometric signals is measured by fast detectors in a real-time regime. Two different detuning of the probe laser from D2 line of Rb was applied, see Fig.2.

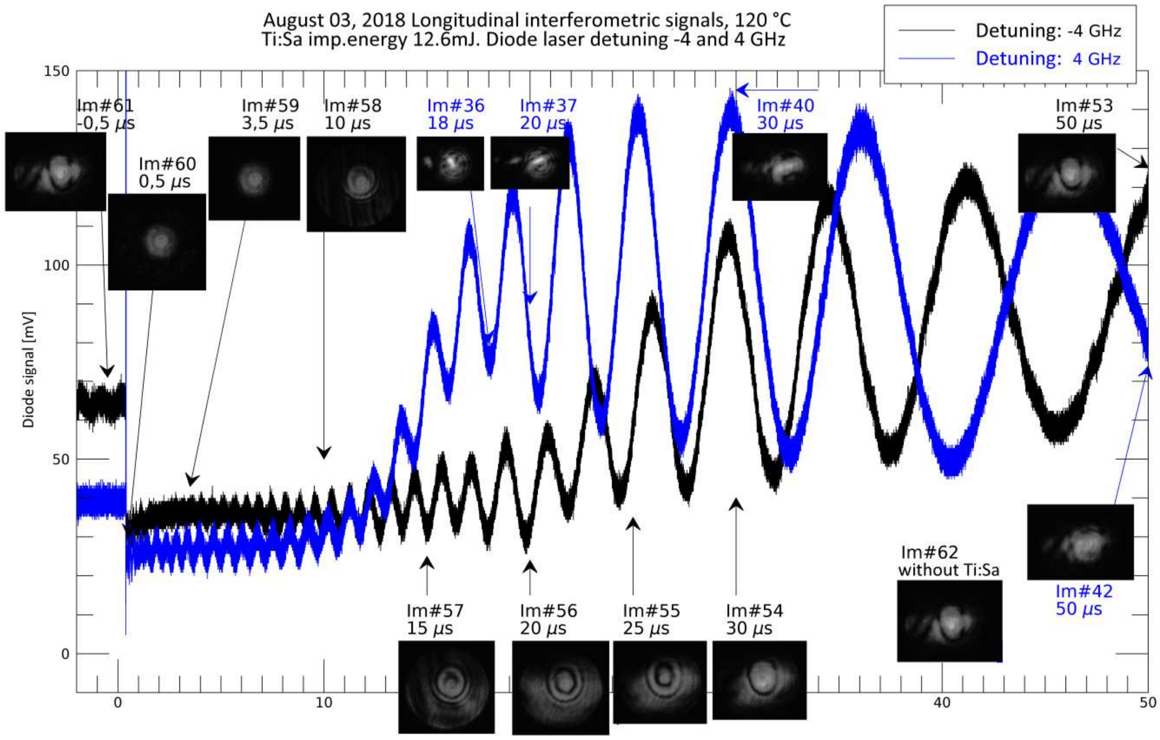


Fig.2. The interferometric signals for negative (black) and positive (blue) detuning of the probe signal along with pictures of the signal beam propagated through the plasma channel.

In one case the frequency of the probe had negative(-4GHz) and in the second case it had positive detuning (4GHz) from the resonant D2 line. The analysis shows that while in the case of the negative detuning, the refractive index of the Rb atoms surrounding the plasma channel is smaller than that in the channel, in the case of the positive detuning; it is larger than that in the channel.

One can anticipate waveguide-like propagation of the probe signal in the plasma channel in the case of negative detuning and contrary, an additional spreading of the probe signal in the case of positive detuning. Such kind of propagation may be seen in Fig.2, where time dependence of the interferometric signals are shown for the two values of the detuning along with the transverse profiles of the signals at different time instances. A waveguide–like propagation of the signal in the plasma channel for the negative detuning is clearly seen due to its structure reminiscent to the waveguide mode structure.

In 2018 we examined, using numerical simulations the phenomenon of pulse propagation in a vapor of atomic rubidium. The ultrashort, resonant laser pulses we considered were intensive enough to ionize the rubidium atoms.

The equations developed for the calculations in recent years that utilized relatively simple, few-level atomic models to calculate the optical response of rubidium were upgraded to use nonlinear envelope equations for the light field that can describe arbitrarily steep pulse fronts that may develop in the nonlinear medium. The improved code was run extensively on the Wigner Cloud computing facility and the solutions analyzed in detail. Self-focusing of the laser pulse was observed for smaller pulse energies and self-channeling of the pulse energy was observed for larger pulse energies. The developing of a plasma channel with 100% ionization of the rubidium atoms was observed, which is an important step in plasma-wakefield accelerator devices such as that being built by the AWAKE collaboration in CERN. The scaling of the plasma channel length and radius with the pulse energy, pulse focusing and vapor density were examined in detail. For the verification of the theoretical results, a comparison of the data provided by the laser propagation measurements of the AWAKE collaboration has begun.

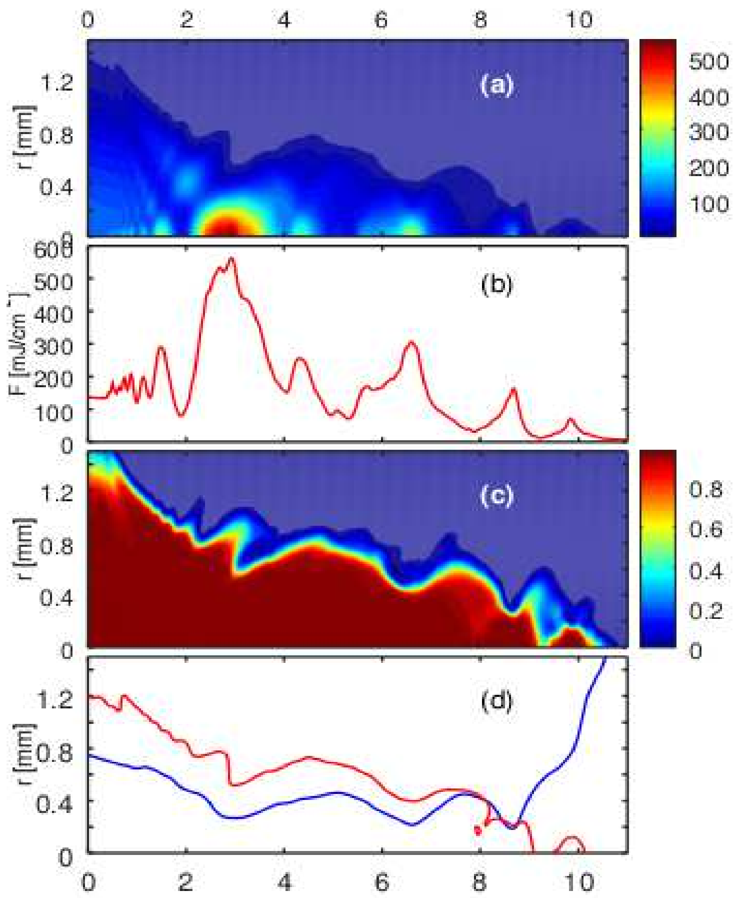


Fig.3.a) Contour plot of radiant fluence (mJ/cm²); b) On axis radiant fluence; c,d) contour plots of ionization probability

Grants and international cooperation

The Excellence Program Grant of the Hungarian Academy of Sciences, III phase (G. Dzsotjan, 2018)

AWAKE Collaboration Agreement, Max Planck Institute for Physics, München, Germany (2015), (contact person: G.P. Dzsotjan)

Agreement of Academic Cooperation between Wigner Research Center and the Yerevan State University (2015-), (contact person: G.P. Dzsotjan)

Collaboration with the Technical University of Kaiserslautern, Kaiserslautern, Germany

Collaboration with the University of Bourgogne, Dijon, France

2018-1.2.1-NKP-2018-00012 Ultrafast experiments for better functional molecules, nanocircuits and atomic beams (NKP-ELI), (Dzsotjan GP, 2018-2022)

MTA INFRA-2018 (Dzsotjan GP)

Publications

Articles

1. Castellini A, Jauslin HR, Rousseaux B, Dzsotján D, Colas des Francs G, Messina A, Guérin S.: Quantum plasmonics with multi-emitters: application to stimulated Raman adiabatic passage. EUR PHYS J D 72:12 223/1-14 (2018)
2. Djotyan GP, Bakos JS, Kedves MÁ, Ráczkevi B, Dzsotján D, Varga-Umbrich K, Sörlei Z, Szigeti J, Ignácz P, Lévai P, Czitrovszky A, Nagy A, Dombi P, Rácz P: Real-time interferometric diagnostics of rubidium plasma. ***NUCL INSTRUM METH A*** **884**: 25-30 (2018)

See also: R-O. W7-X Collaboration 4.

R-M. ITER and fusion diagnostic development

Gábor Veres, Tétény Baross, Livia Beri, Tamás Ilkei, Jenő Kádi, Balázs Leskó, Domokos Nagy, Réka Nagy, József Németh, Miklós Palánkai, László Poszovecz, Bálint Z. Szabó, Gábor Tari, Mátyás Tóth, András Vargyas, Erik Walcz, András Zsákai

Subtitle. — In support of a successful ITER and other fusion oriented projects worldwide.

In 2018, we fully designed and partially manufactured a **new Alkali Beam Injector** for the Plasma Physics Institute in Garching. Several parts of our existing reference design were improved and substantially redesigned. Fig.1 below shows the complex structure of the equipment.

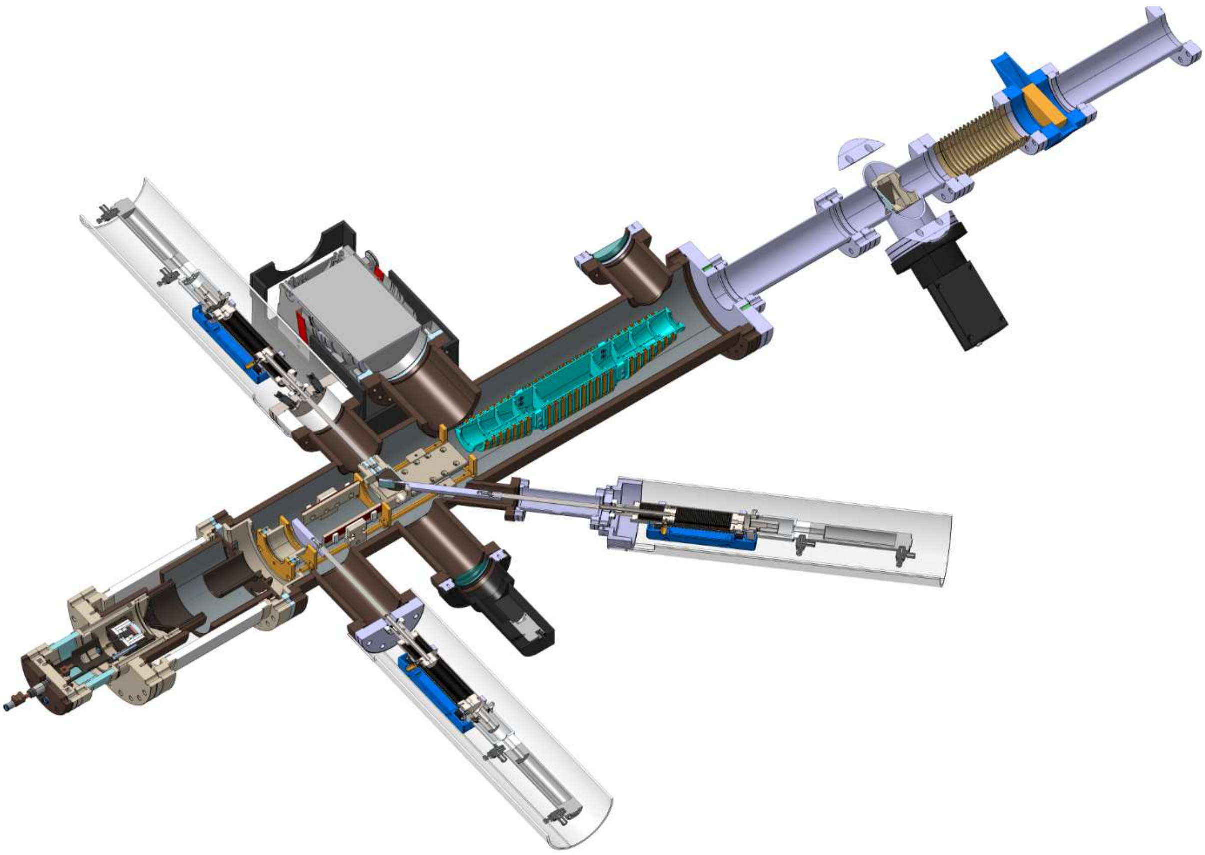


Figure 1: *The Alkali Beam Injector for IPP-Garching*

In the **Tokamak Services for Diagnostics** project that is responsible for the development of the electrical infrastructure for signal transmission in the vacuum vessel, the group continued the series of qualification experiments to qualify the Mineral Insulated (MI) cables for ITER. This year these included vacuum outgassing and vacuum tightness measurements, as well as the characterization of the pulling force of the cables in the looms and thermal conductivity tests of complete assembled loom segments (Fig.2).

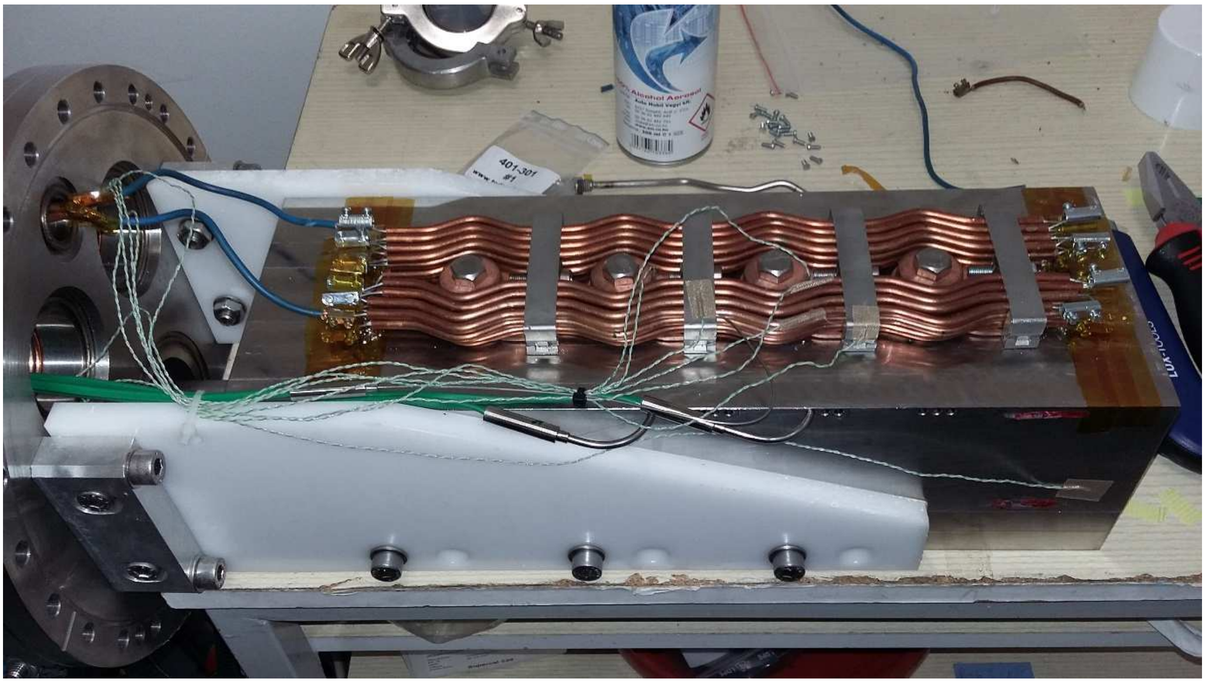


Figure 2: *ITER VV mockup-segment with the installed loom elements*

In the **EUROfusion Consortium** we largely contributed to two work packages: to the WP on the Breeding Blanket (targeting the development of a Tricium breeder unit) and the WP on the Early Neutron Source (targeting the development of a high flux 14 MeV neutron source for fusion material testing).

Grants

F4E-FPA-328 Tokamak Services for Diagnostics (G. Veres, 2012-2018)

F4E-FPA-384 Diagnostic Development: ITER Bolometers (G. Veres, 2014-2018)

F4E-FPA-408 Diagnostic Development: Charge Exchange Resonance Spectroscopy (G. Veres, 2018-22)

EUROfusion (G. Veres, 2014-2020)

International cooperation

Max Planck Institute of Plasma Physics (Garching, Germany), Development of ITER bolometers (G. Veres)

The European Joint Undertaking for ITER and the Development of Fusion Energy (Barcelona, Spain), Tokamak Services (G. Veres)

ITER International Organization (St. Paul-lez-Durance, France), In-vessel Electrical Services (G. Veres)

Publications

Articles

1. Cismondi F et al. incl. Veres G [34 authors]: Progress in EU Breeding Blanket design and integration. ***FUSION ENG DES*** **136**: 782-792 (2018)

2. González-Teodoro JR, Martin P, Edlington T, Martin A, Millot C, Baross T, Palánkai M, Szalardy S, Korossy-khayll A, Nagy D: In vessel electrical integration in ITER—Requirements & solutions. ***FUSION ENG DES*** **127**: 99-105 (2018)

See also: R-O.1, R-O.5, R-O W7-X Collaboration

Anda, G ; Aradi, M ; Asztalos, O ; Bató, S ; Bencze, A ; Berta, M ; Demeter, G ; Dunai, D ; Hacek, P ; Hegedűs, S et al.: Advanced neutral alkali beam diagnostics for applications in fusion research (invited). REVIEW OF SCIENTIFIC INSTRUMENTS 89 : 10 Paper: 10D107 , 9 p. (2018)

See also: R-Q Jet Collaboration ()

R-N. Laser plasma

István B. Földes, Márk Aladi[#], Imre Ferenc Barna, Zsolt Kovács[#], Mihály Pocsai[#]

Spectral interferometry and isolated attosecond pulses. — The interaction of ultra-intense laser pulses with matter opened the way to generate the shortest light pulses available nowadays in the attosecond regime. Ionized solid surfaces, also called plasma mirrors, are promising tools to enhance the potential of attosecond sources in terms of photon energy, photon number and duration especially at relativistic laser intensities. Although the production of isolated attosecond pulses and the understanding of the underlying interactions represent a fundamental step towards the realization of such sources, these are challenging and have not yet been demonstrated. Laser waveform-dependent high-order harmonic radiation was demonstrated in the extreme ultraviolet spectral range supporting well-isolated attosecond pulses, and utilize spectral interferometry to understand its relativistic generation mechanism. This unique interpretation of the measured spectra provides access to unrevealed temporal and spatial properties such as spectral phase difference between attosecond pulses and field-driven plasma surface motion during the process (Fig.1).

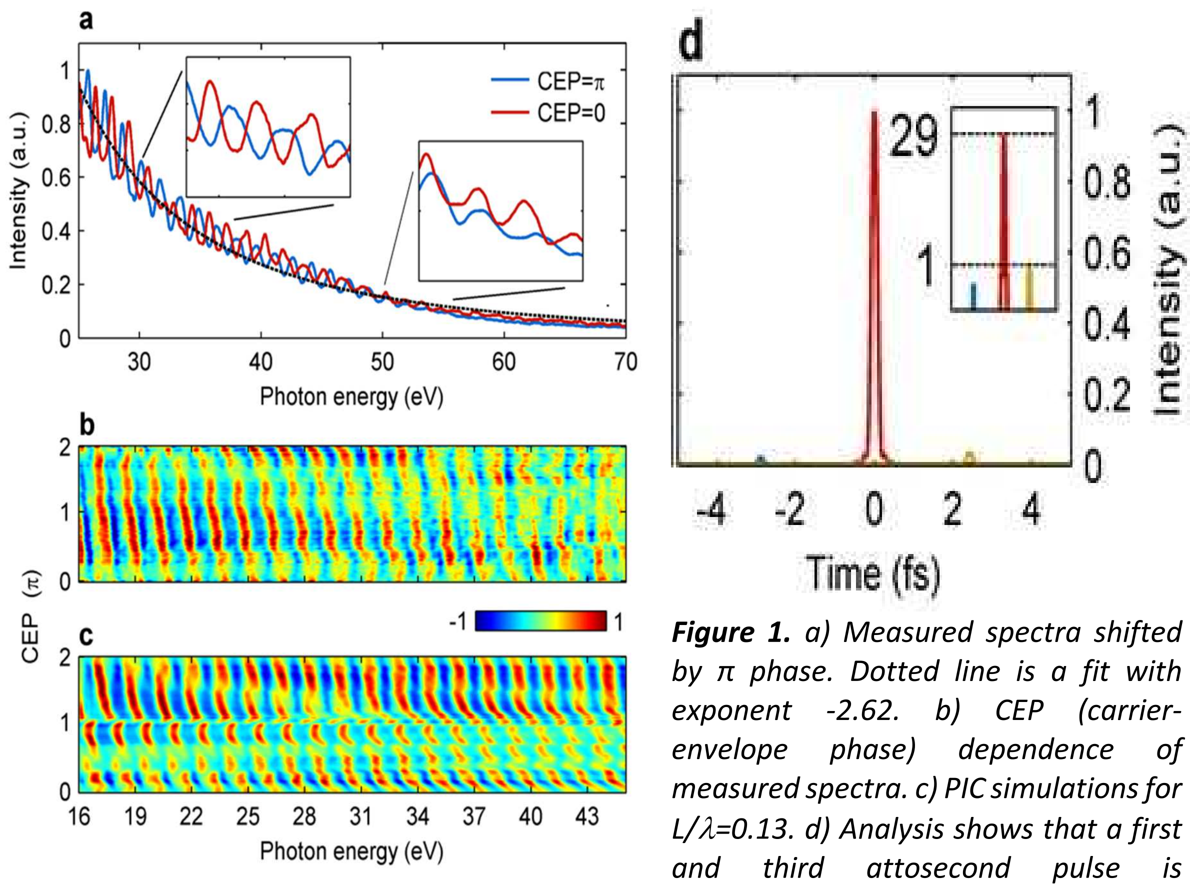
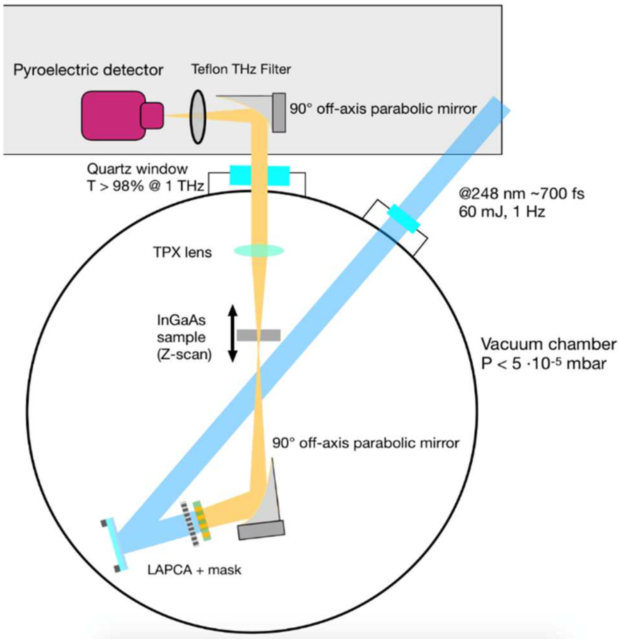


Figure 1. a) Measured spectra shifted by π phase. Dotted line is a fit with exponent -2.62. b) CEP (carrier-envelope phase) dependence of measured spectra. c) PIC simulations for L/λ=0.13. d) Analysis shows that a first and third attosecond pulse is suppressed ~30x for a given CEP value.

Nonlinear effects by THz radiation. — Large-aperture photoconductive antennas (LAPCA) are optically pumped sources of intense THz radiation, generating unique half-cycle THz pulses with strong asymmetry and low frequency components, the latter being advantageous when requiring high ponderomotive potential. The generation of intense electromagnetic waves was studied systematically from wide bandgap LAPCAs (ZnSe, GaN, 6H-SiC, 4H-SiC and β-Ga_2O_3), pumped by KrF laser pulses at 248 nm wavelength, with optical energies up to 80 mJ. The main advantage of working with wide bandgap semiconductor crystal for LAPCAs is that the maximum applied voltage, which determines the maximum radiated peak electric field, is much higher due to the superior breakdown field of the substrate. From the autocorrelation trace, we found that the radiated frequencies are below 0.4 THz with the peak frequency located at 50 GHz, which is sub-THz wave. Also, the maximum measured energy was 11 µJ, which is to date the highest energy from LAPCAs sources, when the 4H-SiC was biased up to 62 kV/cm. By performing Z-scan experiment, we demonstrated a 1.7 times non-linear transmission enhancement inside an n-doped InGaAs layer (Fig.2).



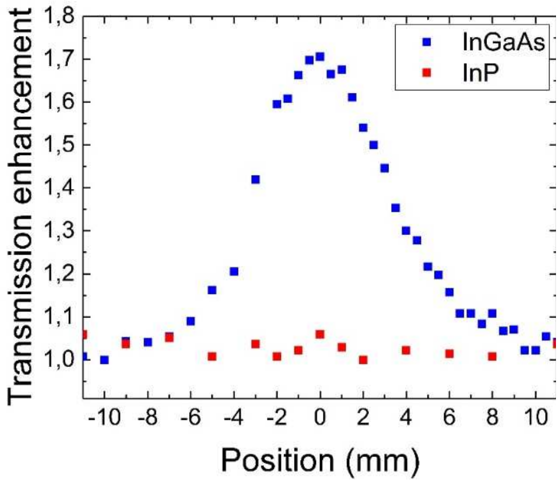


Figure 2. *Experimental arrangement and nonlinear transmission of an InGaAs sample*

Grants

EUROFUSION, Enabling Research ToIFE project, "Preparation and Realization of European Shock Ignition Experiment" project

VEKOP-2.3.2-16 participation

International cooperation

Max Planck Institute of Quantum Optics (MPQ), Garching, Germany.

Institut national de la recherche scientifique (INRS), Montreal, Canada.

IFPILM, Warsaw, Poland.

AWAKE Experiment CERN.

DESY (Hamburg, Germany), EUPRAXIA-Project (Project Head: Ralph Assmann).

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Articles

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2. Barna IF, Pocsai MA, Varró S: The influence of a strong infrared radiation field on the conductance properties of doped semiconductors. ***EUR PHYS J-APPL PHYS*** **84**:2 20101/1-8 (2018)
3. Kormin D, Borot A, Ma G, Dallari W, Bergues B, Aladi M, Földes IB, Veisz L: Spectral interferometry with waveform-dependent relativistic high-order harmonics from plasma surfaces. ***NAT COMMUN*** **9**:1 4992/1-8 (2018)

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See also: S-H.16

R-O. Beam emission spectroscopy

Dániel Dunai, Gábor Anda, Sándor Bató, Attila Bencze, A. Búzás[#], Sándor Hegedűs, Tibor Krizsanóczi, Máté Lampert, Gergő Pokol, Dániel Réfy[#], Balázs Tál, Miklós Vécsei, Sándor Zoletnik

Alkali beam diagnostics measurements on the Wendelstein 7-X stellarator in Germany. — Working in the fusion plasma physics field the Beam Emission Spectroscopy (BES) research group designs, manufactures, installs and operates BES diagnostics in several major fusion devices worldwide. A new alkali beam diagnostic was installed in 2017 on the Wendelstein 7-X (W7-X) stellarator in Greifswald. It was designed to provide high spatially and temporally resolved edge density profiles as well as high frequency measurements for fluctuation characterization. These unique capabilities were utilized in 2018, when the diagnostic was operated by the members of the BES research group during the four months long physics campaign.. With the analysis of the experimental results various edge plasma phenomena were characterized, which gives an important contribution to the understanding of the transport processes in the W7-X stellarator. Another unique capability of the BES diagnostic is that it can measure simultaneously in the scrape off layer plasma, in the edge magnetic islands and in the outer part of the confined plasma. Edge plasma oscillations with about 200 Hz were observed, where the scrape off layer turbulence level and the edge profile gradients were found to be correlated. Edge Localised Mode (ELM) like phenomena was also observed in some specific plasma scenarios. However, in contrast to ELMs in tokamaks the detailed analysis showed that the causing perturbation appears several cm inside the Last Closed Magnetic Surface. Several other physics phenomena have been documented and are being analysed.

Atomic Beam Probe. — Measurement of the plasma edge current density distribution and temporal evolution during the edge localized mode (ELM) cycle is of particular interest in the field of magnetically confined plasmas. To solve this issue a new diagnostic technique called Atomic Beam Probe (ABP) diagnostic is being developed, which is an extension of the alkali BES diagnostic. The project is a joint development with the Institute of Plasma Physics of the CAS in Prague. In this diagnostic ions originated from the diagnostic alkali beam and ionized by the plasma are measured. The high energy ions from the beam are directed to a curved trajectory by the toroidal magnetic field and they can leave the plasma. The poloidal magnetic field of the plasma current deflects the ions toroidally. The location of the passing ion beam carries information on the plasma current distribution. Measuring a few microampere ion current close to the plasma edge requires a special detector. A novel Faraday cup matrix detector utilizing printed-circuit board technology was developed and tested at Wigner for this purpose, which was installed on the COMPASS tokamak in autumn 2018. (*Figure 3*.)

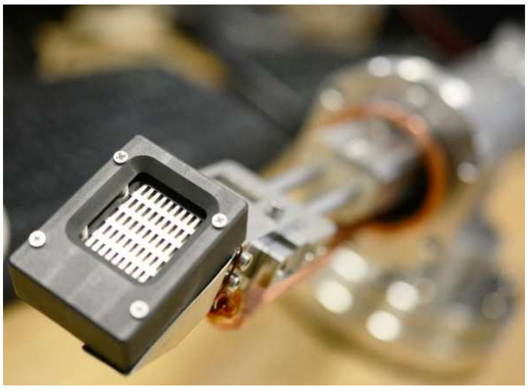

***Figure 3**. Atomic Beam Probe detector head*

In this detector the secondary electrons induced by the plasma radiation and the ion bombardment are inherently confined into the cups by the tokamak magnetic field, and will not cause disturbing offset. Additionally, a double mask is installed in the front face to limit ion influx into the cups and supplement secondary electron suppression. First measurements confirm the basic capabilities of the method.

Scrape-off layer fluctuations on COMPASS. — Recently the lithium Beam Emission Spectroscopy (Li-BES) diagnostic system on COMPASS has reached its full diagnostic power in terms of routine automatic operation in all kinds of plasma scenarios. It is a standard diagnostic for reconstruction of ultrafast density profiles in the edge region of COMPASS plasmas. A detailed study of the diagnostic capability in characterizing plasma fluctuations in various radial regions has been performed. It has been shown how the atomic physics of plasma-beam interaction can affect the interpretation of the measured fluctuating signals at various radial positions. Experimental verification of the stochastic Garcia-model for scrape-off layer filaments and accompanying holes (density deficits) using non-perturbative diagnostic have been demonstrated for the first time using only data acquired by non-perturbative (Li-BES) diagnostic.

Grants

Eurofusion Grants

International cooperation

Culham Centre for Fusion Energy (Culham, UK),

Institute of Plasma Physics (Prague, Czech Rep.),

Max Planck Institute for Plasma Physics (Greifswald, Germany),

Institute of Plasma Physics – ASIPP, (Hefei, China),

National Fusion Research Institute (Daejeon, Korea)

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3. Vécsei M, Dietzel M, Hardt S: Interfacial instability of liquid films coating the walls of a parallel-plate channel and sheared by a gas flow. ***MICROFLUID NANOFLUID* 22**:9 91/1-21 (2018)
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5. Hacek P, Berta M, Anda G, Aradi M, Bencze A, Dunai D, Krbec J, Panek R, Réfy DI, Stockel J, Weinzettl V, Zoletnik S: Development of an ion beam detector for the atomic beam probe diagnostic. ***REV SCI INSTRUM*** **89**:11 113506/1-10 (2018)
6. Grover O, Seidl J, Réfy D, Adamek J, Vondracek P, Tomes M, Junek P, Hacek P, Krbec J, Weinzettl V, Hron M, Zoletnik S and The COMPASS Team: Limit cycle oscillations measurements with Langmuir and ball-pen probes on COMPASS. ***NUCL FUSION*** **58**:11 Paper: 112010 , 12 p. (2018)

JET Collaboration

Due to the vast number of publications of the large collaborations in which the research group participated in 2018, here we list only articles where there are Wigner researchers among the named authors, and also a short selection of appearences in journals with the highest impact factor. According to the list published in X. Litaudon et al., ***NUCL FUSION*** 57:10 102001, 2017, JET Contributors from the Wigner RCP are Bodnár G, Cseh G, Dunai D, Kocsis G, Petravich G, Réfy D, Szabolics T, Tál B, Zoletnik S.

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2. Réfy DI, Brix M, Gomes R, Tál B, Zoletnik S, Dunai D, Kocsis G, Kálvin S, Szabolics T and JET Contributors: Sub-millisecond electron density profile measurement at the JET tokamak with the fast lithium beam emission spectroscopy system. ***REV SCI INSTRUM*** **89**:4 043509/1-8 (2018), Erratum: ***REV SCI INSTRUM*** **89**:6 069902/1-1 (2018)
3. Rzadkiewicz J et al. (JET Contributors): High-resolution tungsten spectroscopy relevant to the diagnostic of high-temperature tokamak plasmas. ***PHYS REV A*** **97**:5 052501/1-9 (2018)
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5. Batistoni P et al. (JET Contributors): 14 MeV calibration of JET neutron detectors-phase 2: in-vessel calibration. ***NUCL FUSION*** **58**:10 106016/1-16 (2018)
6. Bonanomi N et al. (JET Contributors): Turbulent transport stabilization by ICRH minority fast ions in low rotating JET ILW L-mode plasmas. ***NUCL FUSION*** **58**:5 056025/1-11 (2018)
7. Bonanomi N et al. (JET Contributors): Effects of nitrogen seeding on core ion thermal transport in JET ILW L-mode plasmas. ***NUCL FUSION*** **58**:2 026028/1-12 (2018)
8. Bonanomi N et al. (JET Contributors): Light impurity transport in JET ILW L-mode plasmas. ***NUCL FUSION*** **58**:3 036009/1-9 (2018)
9. Bonanomi N et al. (JET Contributors): Impact of electron-scale turbulence and multi-scale interactions in the JET tokamak. ***NUCL FUSION*** **58**:12 124003/1-7 (2018)
10. Bourdelle C et al. (JET Contributors): Fast H isotope and impurity mixing in ion-temperature-gradient turbulence. ***NUCL FUSION*** **58**:7 076028/1-16 (2018)
11. Bowman C et al. (JET Contributors): Pedestal evolution physics in low triangularity JET tokamak discharges with ITER-like wall. ***NUCL FUSION*** **58**:1 016021/1-17 (2018)
12. Breton S et al. (JET Contributors): First principle integrated modeling of multi-channel transport including Tungsten in JET. ***NUCL FUSION*** **58**:9 096003/1-22 (2018)

13. Budny RV and JET Contributors: Alpha heating, isotopic mass, and fast ion effects in deuterium-tritium experiments. ***NUCL FUSION*** **58**:9 096011/1-26 (2018)
14. De Masi G et al. (JET Contributors): Density and magnetic fluctuations in type III-ELM pedestal evolution in JET: experimental and numerical characterization. ***NUCL FUSION*** **58**:4 046007/1-11 (2018)
15. de Vries PC et al. (JET Contributors): Multi-machine analysis of termination scenarios with comparison to simulations of controlled shutdown of ITER discharges. ***NUCL FUSION*** **58**:2 026019/1-13 (2018)
16. Ding BJ et al. (JET Contributors): Review of recent experimental and modeling advances in the understanding of lower hybrid current drive in ITER-relevant regimes. ***NUCL FUSION*** **58**:9 095003/1-17 (2018)
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18. Eich T et al. (ASDEX Upgrade Team and JET Contributors): Correlation of the tokamak H-mode density limit with ballooning stability at the separatrix. ***NUCL FUSION*** **58**:3 034001/1-5 (2018)
19. Faugeras B et al. (JET Contributors): Equilibrium reconstruction at JET using Stokes model for polarimetry. ***NUCL FUSION*** **58**:10 106032/1-19 (2018)
20. Felici F et al. (JET Contributors and EUROfusion MST1 Team): Real-time-capable prediction of temperature and density profiles in a tokamak using RAPTOR and a first-principle-based transport model. ***NUCL FUSION*** **58**:9 096006 , 11 p. (2018)
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22. Giudicotti L et al. (JET Contributors): First observation of the depolarization of Thomson scattering radiation by a fusion plasma. ***NUCL FUSION*** **58**:4 044003/1-6 (2018)
23. Guillemaut C et al. (JET Contributors): Experimental validation of an analytical kinetic model for edge-localized modes in JET-ITER-like wall. ***NUCL FUSION*** **58**:6 066006/1-9 (2018)
24. Hellesen C et al. (JET Contributors): Analysis of resonant fast ion distributions during combined ICRF and NBI heating with transients using neutron emission spectroscopy. ***NUCL FUSION*** **58**:5 056021/1-11 (2018)
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MAST Collaboration

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2. Hnat B, Gadgil S, Kirk A, Militello F, Walkden N and the MAST Team: Experimental constraint on the radial mode number of the geodesic acoustic mode from multi-point Langmuir probe measurements in MAST Ohmic plasma. ***PLASMA PHYS CONTR F*** **60**:8 085016/1-8 (2018)
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4. Saarelma S, Martin-Collar J,; Dickinson D, McMillan BF, Roach CM, MAST Team, JET Contributors: Erratum: Non-local effects on pedestal kinetic ballooning mode stability (2017 Plasma Phys. Control. Fusion 59 064001). ***PLASMA PHYS CONTR F*** **60**:9 099601-1-1 (2018)

TCV Team

1. Maraschek M et al., ASDEX Upgrade team, TCV team and EUROfusion MST1 Team: Path-oriented early reaction to approaching disruptions in ASDEX Upgrade and TCV in view of the future needs for ITER and DEMO. ***PLASMA PHYS CONTR F*** **60**:1 014047/1-11 (2018) (Invited talks from the 44th EPS Conference on Plasma Physics, Belfast, 26-30 June 2017)

See also: R-P ASDEX Upgrade Collaboration (Réfy D, Tál B, Zoletnik S), R-P W7X Collaboration 3, 4, 5,

R-P. Pellet and video diagnostics

Tamás Szepesi, Gábor Cseh[#], Gábor Kocsis, Tamás Szabolics

Video diagnostics system at Wendelstein 7-X (W7-X) — A 10-channel overview video diagnostic system was developed for W7-X superconducting stellarator, based on self-developed Event Detection Intelligent Cameras (EDICAM). During the experimental campaign OP1.2b, spanning from July to October 2018, the system was comprised of eight intelligent EDICAMs and two fast cameras.

One of the fast cameras was used to monitor the injection of carbon-containing pellets (TESPEL). Utilizing these measurements, the time-resolved periodic evolution of pellet clouds was determined. The cloud of the ablating pellet is expanding along magnetic field lines in the 10 microsecond timescale, while it is being ionized. Following this, typically the ionized part of the cloud (a 'cloudlet') is torn off by an instability, and it is leaving the main cloud at a speed in the order of a few km/s. This process is repeated several times until the pellet is completely ablated. The repetitive eruption of cloudlets has a strong effect on the main pellet cloud: following the above cycle, the pattern of the light emitted by the main pellet cloud keeps changing as well. Taking a line cut along the magnetic field line crossing the main cloud (and the pellet), the light intensity profile changes between two distinct states: having one peak centered around the pellet and having two peaks further away from the pellet with a local minimum at the pellet location.

Making use of the line radiation emitted by fuel and impurity particles in the plasma, fast camera measurements with interference filters were also used to determine the magnetic topology of Wendelstein 7-X stellarator in the edge plasma and the islands surrounding the plasma.

In some experiments, the special non-destructive readout mode of the EDICAM cameras was utilized, allowing us to record, simultaneously to the standard overview recoding with 100 frame/s speed, a smaller section Region of Interest (ROI) of the experiment at 50-times higher rate (EDICAM can handle up to six ROIs). Hydrogen pellets, used for increasing the plasma density, arrive at this observed section; the special camera recording allowed for the time-resolved observation of these pellets penetrating and moving inside the plasma.

In long plasma discharges the extended control features of EDICAM were exploited: five ROIs, viewing different areas in the experiment, were defined in several cameras and the readout for these was turned on and off in a controlled manner in order to produce appropriate data for cross-correlation studies about plasma turbulence throughout the plasma discharge, while in the same time, keeping low the amount of data produced.

EDICAM diagnostic development for JT-60SA — The development of a single channel EDICAM system for the world's largest superconducting tokamak, the Japanese JT-60SA, has been started in 2017. The EDICAM, being the first European diagnostic for this experiment, will be part of the overview visible video diagnostic system, monitoring the torus interior from five tangentially viewing channels. In 2018, almost all system components were procured or produced. Minor modifications had to be made to the design, e.g. the camera transport rail was segmented to reduce eddy currents during a disruption. A test environment, featuring a 3.5 m long vacuum chamber, was also established.

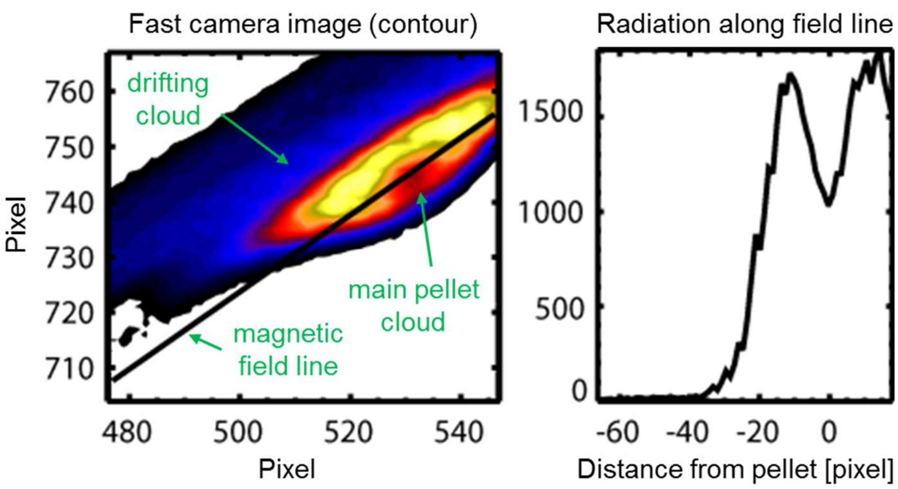

Figure 1. *Left: Fast camera image of an ablating TESPEL pellet. The drifting cloud is shown in blueish color. Right: Light intensity profile along magnetic field line in a time instant where the radiation has a local minimum at the pellet location.*

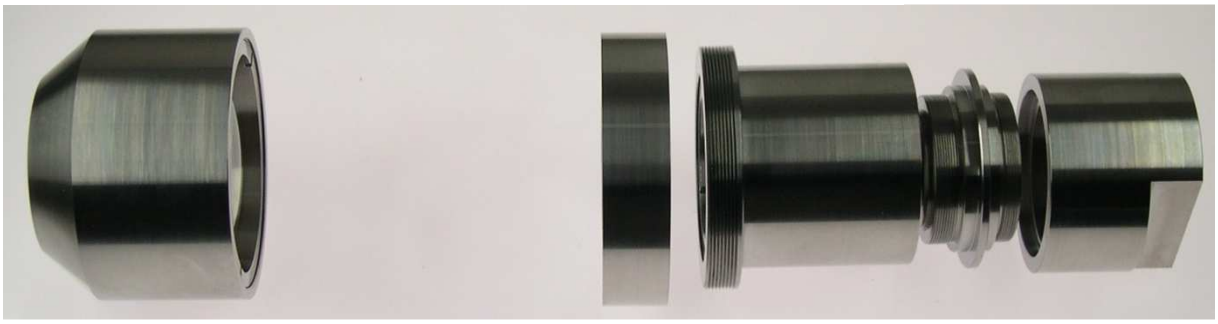

Figure 2. *Optics in stainless steel housing for the JT-60SA EDICAM diagnostic.*

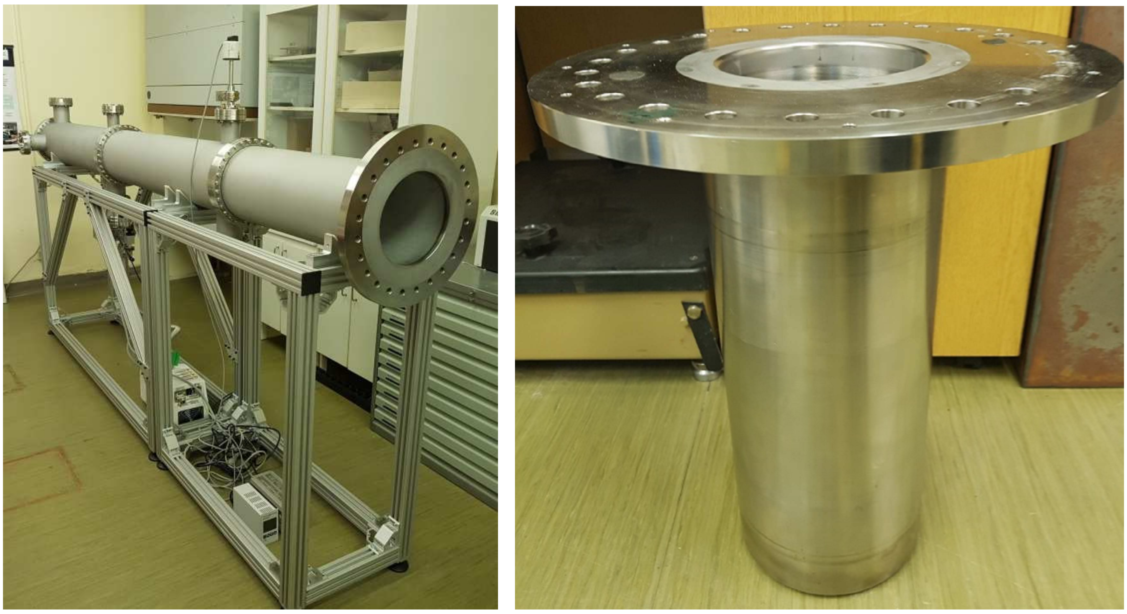

Figure 3. *Left: Vacuum chamber for the testing of the JT-60SA video diagnostic port plug for EDICAM. Right: Mock-up port plug.*

Grants

EUROfusion: WP Medium-Size Tokamak 1 (G. Kocsis, 2017-2018)

EUROfusion: WP Stellarator 1 (G. Kocsis, 2017-2018)

EUROfusion: WP SA (T. Szepesi, 2017-2018)

International cooperation

Max-Planck-Institut für Plasmaphysik, Garching, Germany (G. Kocsis)

Max-Planck-Institut für Plasmaphysik, Teilinstitut Greifswald, Germany (G. Kocsis)

Culham Centre for Fusion Energy, Oxfordshire, UK (G. Kocsis)

National Institutes for Quantum and Radiological Science and Technology, Naka, Japan (T. Szepesi)

Publications

Articles

1. Nagy, R ; Kiraly, M ; Szepesi, T ; Nagy, AG ; Almasi, A: Optical observation of the ballooning and burst of E110 and E110G cladding tubes. NUCLEAR ENGINEERING AND DESIGN 339 pp. 194-201. , 8 p. (2018)
2. Nagy, R. ; Király, M. ; Szepesi, T. ; Nagy, A.G. ; Almási, Á: Optical measurement of the high temperature ballooning of nuclear fuel claddings. REVIEW OF SCIENTIFIC INSTRUMENTS 89 : 12 Paper: 125114 (2018)

See also: R-O.3, R-O.6

ASDEX Upgrade Team

Due to the numerous publications of the large collaborations in which the research group participated in 2018, here we list only articles where there are Wigner researchers among the named authors, and also a short selection of appearences in journals with the highest impact factor. According to A. Kallenbach, ***NUCL FUSON*** **57**: 102015 (2017), Wigner-authors in the ASDEX Upgrade Team are: Cseh G, Erdős B, Kálvin S, Kocsis G, Réfy D, Szepesi T, Tál B, Zoletnik S.

1. Gonzalez-Martin J et al. incl Zoletnik S, Kovacsik A, ASDEX Upgrade team, MST1 Team: First measurements of a scintillator based fast-ion loss detector near the ASDEX Upgrade divertor. ***REV SCI INSTRUM*** **89**:10 10I106/1-5 (2018)
2. Galdon-Quiroga J et al., the ASDEX Upgrade Team, the Eurofusion MST1 Team: Beam-Ion Acceleration during Edge Localized Modes in the ASDEX Upgrade Tokamak. ***PHYS REV LETT*** **121**:2 025002/1-5 (2018)
3. Laggner FM et al., the EUROfusion MST1 Team5 and the ASDEX Upgrade Team: Plasma shaping and its impact on the pedestal of ASDEX Upgrade: edge stability and inter-ELM dynamics at varied triangularity. ***NUCL FUSION*** **58**:4 046008/1-13 (2018)
4. Hornsby WA et al., ASDEX Upgrade Team: Global gyrokinetic simulations of intrinsic rotation in ASDEX Upgrade Ohmic L-mode plasmas. ***NUCL FUSION*** **58**:5 056008/1-14 (2018)

5. Carralero D et al., the ASDEX Upgrade Team and the EURO-fusion MST1: On the role of filaments in perpendicular heat transport at the scrape-off layer. ***NUCL FUSION*** **58**:9 096015/1-13 (2018)
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7. de Vries PC et al., the Alcator C-MOD team, the ASDEX Upgrade team, the DIII-D team, the EAST team, JET contributors, the KSTAR team, the NSTX-U team, the TCV team and ITPA IOS members and experts: Multi-machine analysis of termination scenarios with comparison to simulations of controlled shutdown of ITER discharges. ***NUCL FUSION*** **58**:2 026019/1-13 (2018)
8. Galdon-Quiroga J et al., the ASDEX Upgrade Team and the EUROfusion MST1 Team: Velocity space resolved absolute measurement of fast ion losses induced by a tearing mode in the ASDEX Upgrade tokamak. ***NUCL FUSION*** **58**:3 036005/1-7 (2018)
9. Guimarais L et al., the ASDEX Upgrade Team and the EUROfusion MST1 Team: Poloidal asymmetries in the edge density profiles on ASDEX Upgrade. ***NUCL FUSION*** **58**:2 026005/1-13 (2018)
10. Harrer GF et al., the EUROfusion MST1 Team and the ASDEX Upgrade Team: Parameter dependences of small edge localized modes (ELMs). ***NUCL FUSION*** **58**:11 112001/1-10 (2018)
11. Henderson SS et al., the ASDEX Upgrade Team and the MST1 Team: Determination of volumetric plasma parameters from spectroscopic N II and N III line ratio measurements in the ASDEX Upgrade divertor. ***NUCL FUSION*** **58**:1 016047/1-10 (2018)
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13. Krieger K et al., ASDEX-Upgrade Team and EUROfusion MST1 Team: Experiments on transient melting of tungsten by ELMs in ASDEX Upgrade. ***NUCL FUSION*** **58**:2 026024/1-19 (2018)
14. Lebschy A et al., ASDEX Upgrade Team: Measurement of the complete core plasma flow across the LOC-SOC transition at ASDEX Upgrade. ***NUCL FUSION*** **58**:2 026013/1-12 (2018)
15. Mink AF et al., ASDEX Upgrade Team: Nonlinear coupling induced toroidal structure of edge localized modes. ***NUCL FUSION*** **58**:2 026011/1-7 (2018)
16. Plyusnin VV et al., COMPASS team, TCV team, ASDEX-Upgrade team, EUROFusion MST1 Team and JET contributors: Comparison of runaway electron generation parameters in small, medium-sized and large tokamaks-A survey of experiments in COMPASS, TCV, ASDEX-Upgrade and JET. ***NUCL FUSION*** **58**:1 016014/1-15 (2018)
17. Ratynskaia S et al., the ASDEX-Upgrade Team and the EUROfusion MST1 Team: Interaction of metal dust adhered on castellated substrates with the ELMy H-mode plasmas of ASDEX-Upgrade. ***NUCL FUSION*** **58**:10 106023/1-14 (2018)
18. Salewski M et al., the EUROfusion MST1 team and the ASDEX Upgrade team: Deuterium temperature, drift velocity, and density measurements in non-Maxwellian plasmas at ASDEX Upgrade. ***NUCL FUSION*** **58**:3 036017/1-12 (2018)

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20. Sips ACC et al., JET Contributors, the ASDEX Upgrade team, the DIII-D team, the C-Mod team, the JT-60U team and ITPA-IOS TG members and experts: Assessment of the baseline scenario at q_{95} ~ 3 for ITER. ***NUCL FUSION*** **58**:12 126010/1-23 (2018)
21. Vanovac B et al., the ASDEX Upgrade Team: Characterization of low-frequency inter-ELM modes of H-mode discharges at ASDEX Upgrade. ***NUCL FUSION*** **58**:11 112011/1-10 (2018)
22. Viezzer E et al., the ASDEX Upgrade Team and the EUROfusion MST1 Team: Ion heat transport dynamics during edge localized mode cycles at ASDEX Upgrade. ***NUCL FUSION*** **58**:2 026031/1-9 (2018)
23. Weiland M et al., the ASDEX Upgrade Team and the Eurofusion MST1 Team: RABBIT: Real-time simulation of the NBI fast-ion distribution. NUCL FUSION 58:8 082032/1-21 (2018)
24. Prisiazhniuk D et al., the ASDEX Upgrade Team: Density fluctuation correlation measurements in ASDEX Upgrade using poloidal and radial correlation reflectometry. ***PLASMA PHYS CONTR F*** **60**:7 075003/1-18 (2018)
25. Pan O et al., the ASDEX Upgrade Team: SOLPS simulations of detachment in a snowflake configuration for the future upper divertor in ASDEX Upgrade. ***PLASMA PHYS CONTR F*** **60**:8 085005/1-6 (2018)

W7X Collaboration

Due to the numerous publications of the large collaboration in which the research group participated in 2018, here we list only articles where there are Wigner researchers among the named authors, and also a short selection of appearances in journals with the highest impact factor. Unnamed Wigner authors in the collaboration are: Cseh G, Kocsis G, Szabolics T, Szepesi T

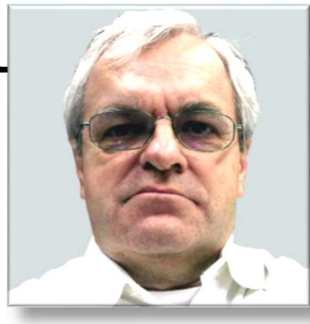
1. Dinklage A et al. incl. Ilkei T, Kocsis G, the W7-X Team: Magnetic configuration effects on the Wendelstein 7-X stellarator. ***NATURE PHYSICS*** **14**: 855–860 (2018), Author Correction: ***NATURE PHYSICS*** **14:** 867 (2018)
2. Wenzel U, Biedermann C, Kocsis G, Szepesi T, Blackwell BD, Klose S, Knauer J, Krychowiak M, Stephey L, Schmitz O, Harris J, König R, Pedersen TS, the W7-X Team: Observation of Marfes in the Wendelstein 7-X stellarator with inboard limiters. ***NUCL FUSION*** **58**:9 096025/1-11 (2018)
3. Hathiramani D et al. incl Anda G, Kocsis G, Szepesi T, Tóth M, Zoletnik S, the W7-X Team: Upgrades of edge, divertor and scrape-off layer diagnostics of W7-X for OP1.2. ***FUSION ENG DES*** **136:** 304-308 (2018)
4. Zoletnik S, Anda G, Aradi M, Asztalos O, Bató S, Bencze A, Berta M, Demeter G, Dunai D, Hacek P, Hegedűs S, Hu GH, Krizsanóczi T, Lampert M, Nagy D, Németh J, Otte M, Petravich G, Pokol GI, Réfy D, Tál B, Vécsei M, and W7-X Team: Advanced neutral alkali beam diagnostics for applications in fusion research. ***REV SCI INSTRUM*** **89**:10 10D107/1-9 (2018)

5. Zoletnik S, Biedermann C, Cseh G, Kocsis G, König R, Szabolics T, Szepesi T, the W7-X Team: First results of the multi-purpose real-time processing video camera system on the Wendelstein 7-X stellarator and implications for future devices. ***REV SCI INSTRUM*** **89**:1 013502/1-10 (2018)
6. Wegner Th et al. incl. Cseh G, Kocsis G, Szepesi T, W7-X Team: Design, capabilities, and first results of the new laser blow-off system on Wendelstein 7-X. ***REV SCI INSTRUM*** **89**:7 073505/1-5 (2018)
7. Sitjes AP et al. incl. Kocsis G, Szepesi T, Szabolics T, the W7-X Team: Wendelstein 7-X near real-time image diagnostic system for plasma-facing components protection. ***FUSION SCI TECHNOL*** **74**:1-2 116-124 (2018)
8. Boeckenhoff D et al., the W7-X Team: Reconstruction of magnetic configurations in W7-X using artificial neural networks. **NUCL FUSION 58**:5 056009/1-10 (2018)
9. Liu, SC et al., the W7-X Team: Observations of the effects of magnetic topology on the SOL characteristics of an electromagnetic coherent mode in the first experimental campaign of W7-X. ***NUCL FUSION*** **58**:4 046002/1-12 (2018)
10. Lobsien J-F et al., the W7-X Team: Stellarator coil optimization towards higher engineering tolerances. ***NUCL FUSION*** **58**:10 106013/1-8 (2018)
11. Panadero N et al., the W7-X team: Experimental studies and simulations of hydrogen pellet ablation in the stellarator TJ-II. ***NUCL FUSION*** **58**:2 026025/1-19 (2018)
12. Sinha P et al., the W7-X Team: Numerical studies of scrape-off layer connection length in Wendelstein7-X. ***NUCL FUSION*** **58**:1 016027/1-5 (2018)
13. Baldzuhn J et al., the LHD Experiment group, the W7-X Team: Particle fueling experiments with a series of pellets in LHD. ***PLASMA PHYS CONTR F*** **60**:3 035006/1-11 (2018)
14. Garcia-Regana JMet al., the TJ-II Team, the W7-X Team: On-surface potential and radial electric field variations in electron root stellarator plasmas. ***PLASMA PHYS CONTR F*** **60**:10 104002/1-14 (2018)
15. Gradic D et al., the ASDEX Upgrade Team, the W7-X Team, the Eurofusion MST1 team: Doppler coherence imaging of divertor and SOL flows in ASDEX upgrade and Wendelstein 7-X. ***PLASMA PHYS CONTR F*** **60**:8 084007/1-12 (2018)
16. Pablant NA et al., W7-X Team: Core radial electric field and transport in Wendelstein 7-X plasmas. ***PHYS PLASMAS*** **25**:2 022508/1-7 (2018)
17. Dumke S et al., the W7-X team: Next generation web based live data monitoring for W7-X. ***FUSION ENG DES*** **129**: 16-23 (2018)
18. Fellinger J et al., the W7-X Team: Overview of fatigue life assessment of baffles in Wendelstein 7-X. ***FUSION ENG DES*** **136:** 292-297 (2018)
19. Krom JG et al., the W7-X Team: Compression of time-vectors in W7-X archived measurements. ***FUSION ENG DES*** **129:** 326-329 (2018)
20. Schacht J et al., the W7-X Team: The gas supply and gas inlet control systems of the fusion experiment Wendelstein 7-X. ***FUSION ENG DES*** **129:** 6-11 (2018)
21. Pasch E et a., the W7-X Team: Dual-laser wavelength Thomson scattering at Wendelstein 7-X. ***REV SCI INSTRUM*** **89**:10 10C115/1-5 (2018)

22. Pisano F et al., the W7-X Team: Towards a new image processing system at Wendelstein 7-X: From spatial calibration to characterization of thermal events. ***REV SCI INSTRUM*** **89**:12 123503/1-10 (2018)
23. Wurden GA et al., the W7-X Team: A divertor scraper observation system for the Wendelstein 7-X stellarator. ***REV SCI INSTRUM*** **89**:10 10E102/1-5 (2018)
24. Brunner KJ et al., the W7-X Team: Real-time dispersion interferometry for density feedback in fusion devices. ***J INSTRUM*** **13**: P09002/1-21 (2018)
25. Boscary J et al., the W7-X Team: Design and test of Wendelstein 7-X water-cooled divertor scraper. ***IEEE T PLASMA SCI*** **46**:5 1398-1401 (2018)

See also: R-O JET Collaboration (Cseh G, Kocsis G, Szabolics T)

R-R. Space technology



János Zoltán Nagy, András Balázs, Attila Baksa, Lajos Dinnyés[#], László Hevesi, István Horváth, Zoltán Pálos, Bálint Sódor, Sándor Szabó, Lajos Szalai, Sándor Szalai[E], Gábor Tróznai, Pál Gábor Vizi[#]

We are participating in the ESA Juice project, which will arrive at Jupiter in 2030, eight years after its start in 2022. It will take measurements for two years around Jupiter. We develop high-reliability power supply units, DCC (direct current converter) for this program. The goal of the DCC is to ensure power for redundant DPU and 4 sensors of PEP experiment. After several meetings and discussions, our preliminary plans to realize the job was accepted by PEP team. Fig. 1 shows the EM1 model (engineering model). Its goal was to make a working model for integration of EM version of PEP instrument. The EM1 after detailed tests worked correctly. In 2018 we delivered EM1 model for integration ongoing tests in Kiruna. Fig. 2 shows separate DCC for a sensor called JDC developed by our team. .

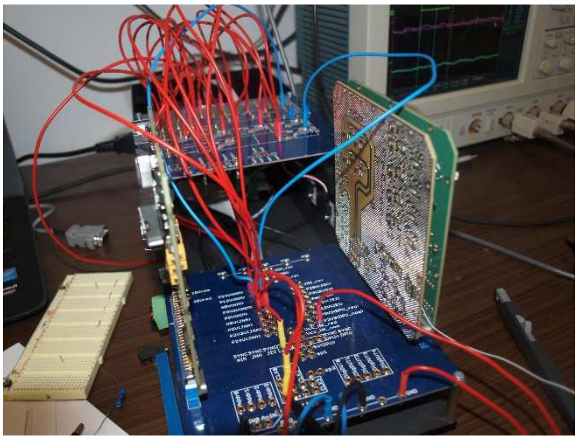


***Figure 1**. The EM1 model of DCC is under testing.*

***Figure 2**. DCC for JDC sensor.*

BepiColombo launched on Ariane-5 launcher from the Kourou Space Center on October 20 at 3:45 AM. The target of the spacecraft is Mercury. Two separate units, the European MPO (Mercury Planetary Orbiter) and the Japanese Mio (also known as Mercury Magnetospheric Orbiter, MMO), will be on track in 2025 around the Inner Planet of the Solar System. We participated in the development of the PICAM (Planetary Ion CAMera) ion-mass spectrometer in this project. The Picam acts as a camera for charged particles to study the chain of surface ionization processes. Our team's engineers have developed the PICAM low voltage power supply and the BepiColombo space probe simulation environment with the involvement of SGF.

Grants

ESA PRODEX: Design, Manufactruring, Validation and Test of Direct Current Converter (DCC) and EGSEs for PEP/JUICE International cooperation (2017-2019)

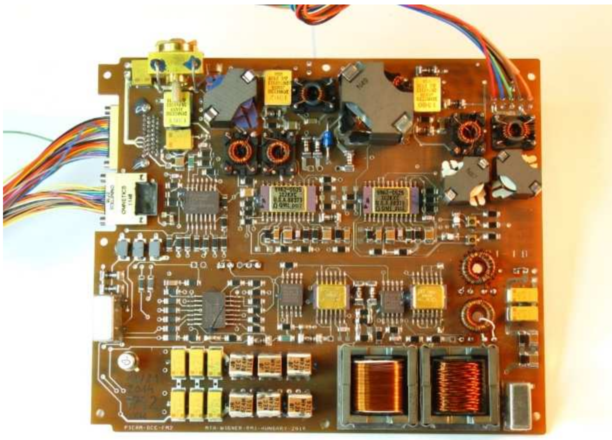


Figure 3. The engineering model of Picam power supply unit.

400123264: Development of Electrical Ground Support Equipment (EGSE) for J-MAG Instrument of Juice

NFM IKF742/2017-NFM:SZERZ Chibis-AI-space weather microsatellite and Obsztanovka-Phase 2 on ISS (2017-2018)

NFM IKF/ 695 /2017-NFM_SZERZ STRANNIK microsatellite configuration (2017-2018)

ESA-EMITS -4000120190 Solar Orbiter (2017-2019)

International cooperation

IRF (Swedish Institute of Space Physics, Kiruna)

IKI Space Research Institute of the Russian Academy of Sciences, Moscow, Russia

Publications

Article

1. Balázs A: A comet revisited: Lessons learned from Philae's landing. ***IEEE SOFTWARE* 35**:4 89-93 (2018)

R-T. Theoretical neuroscience and complex systems

Zoltán Somogyvári, Fülöp Bazsó, Zsigmond Benkő[#], Dorottya Cserpán[#], Péter Érdi[E], Bálint File, János Heszberger, Tamás Kiss, László Négyessy, Marcel Stippinger, László Zalányi

Subtitle. — Analysis of complex systems in the brain and beyond

We showed by using 3D electron microscopic reconstructions and quantitative comparisons that each pathways of the hierarchical circuitry of the somatosensory cortex forms two kinds of synaptic contacts: one exhibiting structural properties, which permit signal transmission at high fidelity, and another with morphological properties of the modulatory type. These findings are crucial in understanding the dynamics of interactions of the different hierarchically organized cortical pathways. The manuscript summarizing these findings is about submission.

The directed interactions have been determined among the variables of a lake ecosystem, via a new causality analysis method. Causality analysis indicated that the observed eutrophication signals were induced by climate change, which altered the phosphate, the fito- and the zooplacton interactions.

A new data analysis method has been developed to generate an electric imaging, based on parallel recordings on intrinsic optical and local field potential by a transparent electrode array. The new method makes possible the fusion of the two methods, by exploiting the advantages of bot, the excellent spatial resolution of the optical imaging and the excellent temporal resolution of the electric signal (Fig. 1).

Schizophrenia is a chronic and severe mental disorder that affects how a person thinks, feels, and behaves, putting significant burden on caregivers and society. The goal of our research is to identify druggable molecular targets in a hope to ameliorate the life of people suffering from this disease. A new project targeting the fundamental question of molecular, system and functional level causes of Schizophrenia was started in 2018 in collaboration with Semmelweis University funded by Gedeon Richter Plc. During this year a new experimental laboratory was set up and preliminary results generated to elaborate on a possible role of NR2C containing NMDA receptors in generating sleep disturbances underlying decreased memory performance, a key symptom of Schizophrenia.

Grants

NKFIH OTKA K-113145, Micro-electric imaging: modeling, source reconstruction and causality analysis for multi-electrode arrays. (Z. Somogyvári, 2015-2018)

ERA-NET FLAG-ERA, Human Brain Project, NKFIH NN-118902: "CANON – Investigating the canonical organization of neocortical circuits for sensory integration". (L Négyessy & Z Somogyvári, 2016-2018)

NIH: „Neural basis of tactile object perception in SI cortex" (consortial subaward to L Négyessy, 1R01NS093998-01A1, 2016-2019)

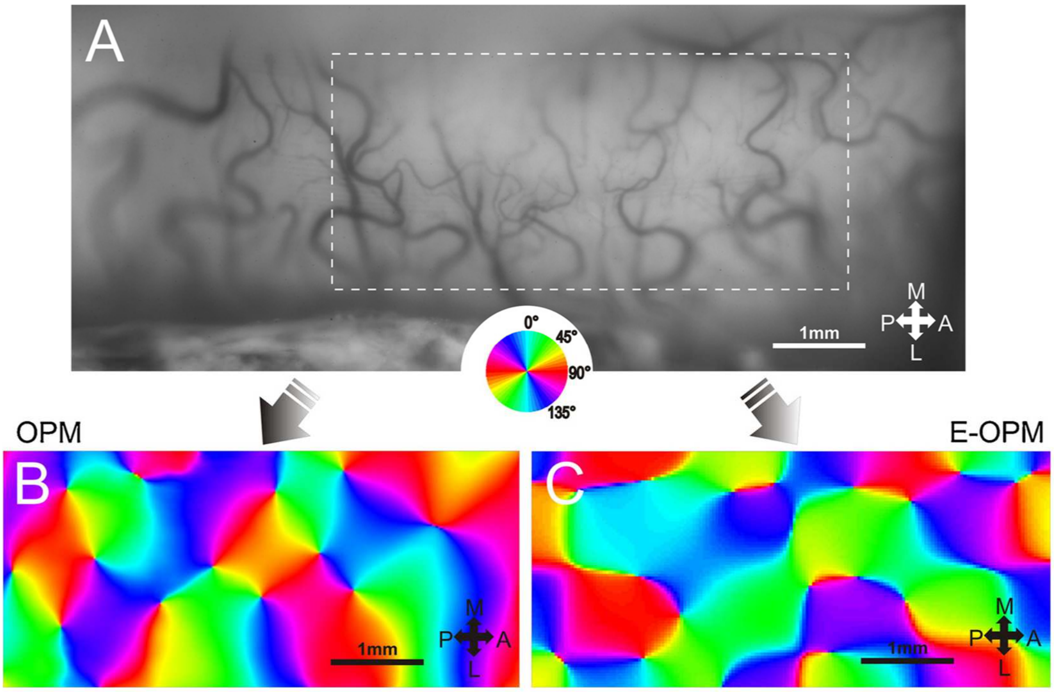


Figure 1. *Comparison between optically and electrically derived orientation preference maps. The white dashed frame on the grayscale vascular image (A) shows the position of the 32-channel microelectrode array inside the investigated A17 region. Traditionally processed orientation preference map (B) and electrical orientation preference map derived from the evoked ECoG responses to the visual stimuli (C) are shown.*

RG-IPI-2017 TP11/13: Investigating the neuropsychiatric role of NR2C subunit containing NMDA receptors (T. Kiss, 2017-).

International cooperations

VTT Technical Research Centre of Finland (Espoo, Finland), Regular structure in networks and graphs (H. Reittu – F. Bazsó)

Oregon Health & Sciences University, (Portland, OR, USA) és Interdisciplinary Institute of Neuroscience and Technology Yuquan Campus, Zhejiang University (38 Zheda Road, Hangzhou, Zhejiang, China) Imaging and mapping sensorimotor circuits in the primate (A. Wang Roe – L. Négyessy).

Neuroscience Research Unit, Pfizer Global Research and Development, Cambridge, MA, USA. Tau-pathology in Alzheimer's disease (L. Scott – T. Kiss)

Translational Neuropharmacology, Section of Comparative Medicine, Yale University School of Medicine, New Haven, CT 06520, USA. Tau-pathology in Alzheimer's disease (M. Hajós – T. Kiss)

Swammerdam Institute for Life Sciences, Universiteit van Amsterdam, Netherland. Investigating the canonical organization of neocortical circuits for sensory integration (C. Bosman and U. Olcese – L. Négyessy, Z. Somogyvári)

Institut national de la santé et de la recherche médicale, INSERM, Lyon, France. Investigating the canonical organization of neocortical circuits for sensory integration (L. Gentet – L. Négyessy, Z. Somogyvári)

Danish Research Institute of Translational Neuroscience, DANDRITE, Aarhus, Danish Kingdom. Electrophysiological recordings and manipulation of single neurons in behaving animals (D. Kvitsiani – Z. Somogyvári)

Center for Complex Systems Studies, Kalamazoo College, 1200 Academy Street, Kalamazoo, MI, USA (P. Érdi)

Swammerdam Institute for Life Sciences, University of Amsterdam, Amsterdam, The Netherlands (U. Olcese, C. Bosman — L. Négyessy, Z. Somogyvári)

Department of Mathematical Sciences, University of Montana, Missoula, MT, 59812, USA (C. Palmer — L. Négyessy)

Department of Neuroanatomy, Faculty of Medicine, Institute of Anatomy and Cell Biology, Albert-Ludwigs-University Freiburg, 79104, Freiburg, Germany (R. Nitschke, O. Kántor — Z. Somogyvári)

Division of Biology and Biological Engineering, California Institute of Technology, Pasadena, CA, 91125, USA (M. Ashaber — L. Négyessy,)

Tufts University, Boston Ave, Medford, MA 02155, USA (B. Tracey — T. Kiss)

Department of Experimental Limnology, Leibniz-Institute of Freshwater Ecology and Inland Fisheries, Stechlin, Germany (L. Krienitz, P. Kasprzak, P. Casper — Z. Somogyvári)

Department of Surgery and Transplantation, University Hospital Zurich, Switzerland, (M. Buetler — B. File)

Human-Centered Engineering Institute of Applied Sciences, Biel, Switzerland, (J. Justiz — B. File)

Department of Psychology and Program in Neuroscience, Florida State University, Tallahassee, FL, USA (A.C. Spector — B. File)

Publications

Articles

1. Kántor O, Szarka G, Benkő Z, Somogyvári Z, Pálfi E, Baksa G, Rácz G, Nitschke R, Debertin G, Völgyi B: Strategic positioning of connexin36 gap junctions across human retinal ganglion cell dendritic arbors. ***FRONT CELL NEUROSCI*** **12**: 409/1-14 (2018)
2. Pálfi E, Zalányi L, Ashaber M, Palmer C, Kántor O, Roe AW, Friedman RM, Négyessy L: Connectivity of neuronal populations within and between areas of primate somatosensory cortex. ***BRAIN STRUCT FUNCT*** **223**:6 2949-2971 (2018)
3. Ujfalussy BB, Makara JK, Lengyel M, Branco T: Global and multiplexed dendritic computations under In vivo-like conditions. NEURON 100:3 579-592 (2018)
4. Vágó L, Ujfalussy BB: Robust and efficient coding with grid cells. ***PLOS COMPUT BIOL*** **14**:1 e1005922/1-18 (2018)

R-U. Neurorehabilitation and motor control

József Laczkó, Szabolcs Malik, Mariann Mravcsik, Lilla Botzheim[#],
István Zsenák[#], Arató, Andras[A]

A graph based dimension reduction method was proposed for analyz assessed from human arm movements. This analysis was performed i University of Pecs and the HAS Wigner Cloud service. The comb dimension reduction method was applied to locate 1-dimensional subspaces in high dimensional task specific kinematic spaces. Identifying such subspaces, it can be shown that which variables can be controlled together by one common centrally controlled parameter. This method has been validated, by applying it to arm cycling. Particularly, kinematic variables (certain coordinates of markers placed on the arm) were identified whose time series differed only in amplitude. This may help to simplify the control of motor tasks.

Lower limb cycling movements were generated for paralysed individuals in the National Institute for Medical Rehabilitation during the year twice a week, using functional electrical muscle stimulation. These cycling and tricycling trainings for spinal cord injured (SCI) people was provided by the research group. Accomplishing functional electrical stimulation driven tricycling trainings for lower limb paralyzed SCI persons, it was shown that cycling speed increased during the series of trainings. This demonstrates the significance of the neurorehabilitation technique applied by the group in cooperation with the Centre for Medical Physics and biomedical Engineering of the Medical University of Vienna (Fig 1).

Arm cycling movements of able-bodied persons were analyzed. The dependence of movement smoothness, jerkiness on joint angular velocities and accelerations was shown for arm cranking movements. The comparison of this result, with results previously found for reaching arm movements, supports the task specificity of smoothness and jerkiness of human movements.

The FES driven cycling movements (as a neuroprosthesis) for new paralyzed users and the TalkPad speech replacement system (as a speech prosthesis) became available for new autistic users as a result of the work of the research group.

International cooperations

Medical University Vienna, Center for Medical Physics and Biomedical Technics (Wien Austria), Functional Electrical Stimulation Driven cycling for lower limb paralyzed persons, (Jozsef Laczko, Wigner RCP)

Shirley Ryan Ability Laboratory (former Rehabilitation Institute of Chicago, Chicago IL, USA), Studying movement coordination deficits after stroke, and body-machine interfaces after spinal cord injury, (Jozsef Laczko, Wigner RCP)

Neural Rehabilitation Group, Cajal Institute, Spanish National Research Council (Madrid, Spain), Muscle synergies in cycling movements, (Jozsef Laczko, Wigner RCP)

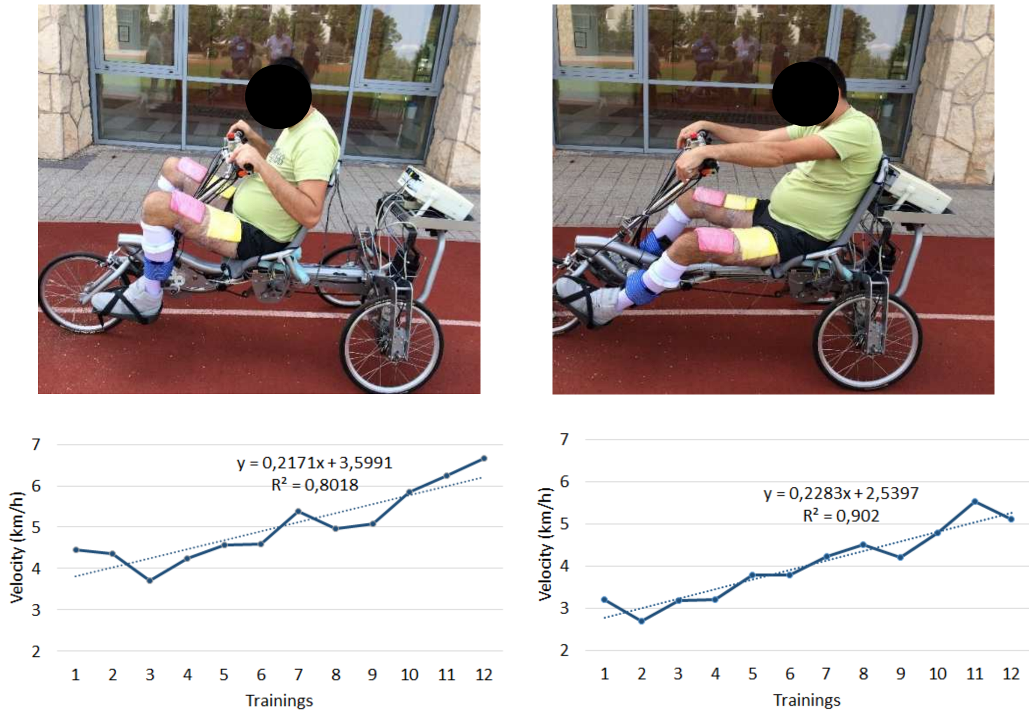


Figure 1. *Tricycling of lower limb paralyzed spinal cord injured individuals, applying functional electrical muscle stimulation for knee extension. Bilateral knee extension starts and actively drives the tricycle as the quadriceps muscles are stimulated (upper left picture). At the end of quadriceps stimulation (at the end of knee extension), start of "rowing mode" when the person starts to pull his body forward by his arm (upper right picture). The speed in 12 consecutive trainings of 2 spinal cord injured, paralyzed participants (lower diagrams): cycling speed increased during the series of trainings.*

Publications

Conference proceeding

1. Mravcsik M, Kast C, Vargas LJL, Aramphianlert W, Hofer C, Malik Sz, Putz M, Mayr W, Laczkó J: FES driven cycling by denervated muscles. In: *Proc. 22th Anual Conference of the Functional Electrical Stimulation Society IFESS2018, Swiss Paraplegic-Centre Nottwil, Switzerland, 29-31 August 2018* (2018) pp. 134-136

Book, book chapter

R-V. Data and Compute Intensive Sciences

István Csabai[A], Máté Ferenc Nagy-Egri, Gábor Vattay[A], Sándor Laki[A], Bálint Pataki[#]

Subtitle. — Machine learning and data analytics platform for infectious disease genetics.

Our group's focus is to foster research in data and computation intensive research areas. The last two decades have seen an unprecedented change in almost all areas of sciences. Before that, most disciplines were determined by the scarcity of experimental data. The exponential pace of microelectronics development has changed this, on one hand by making available high throughput sensors and digital instruments and on the other by providing high-speed computers with large storage and fast interconnecting network. Beyond the almost limitless opportunities, there are demanding challenges, too: how to handle the data avalanche from experiments, how to get out the most from information technology in various scientific disciplines, and also how to understand and manages the ever growing complexity of the computational system itself. We study computer networks and systems like it was a "natural phenomena" and also with continuously following the technologies, we use them for analyzing science data in various fields from genomics to cosmology.

We are part of a large European H2020 project, COMPARE in which bioinformatics tools are developed for outbreak detection. The health of humans and animals around the world is increasingly under threat due to new and recurring epidemics and foodborne disease outbreaks, which place pressure on health services and the production of livestock. These epidemics also reduce consumer confidence in food and negatively impact trade and food security. The longer it takes from the start of an outbreak of for example Ebola, influenza or salmonella until it is detected and stopped, the greater the consequences. The most important factor in being able to limit the consequences and costs of such outbreaks is the ability to quickly identify the disease-causing microorganisms that are causing the disease. Also, there is the need for knowledge about the mechanisms that cause the disease, and how the bacteria are transmitted to and between humans. The goal of the COMPARE project is a better surveillance system for infectious diseases, to speed up the detection of and response to disease outbreaks among humans and animals worldwide using new genome technology. Our group is responsible for the advanced database and data analysis system, which will store, analyse and share the genomic data collected by researchers all over the world. We develop a "virtual research environment", where interested partners can log in, and use the already installed tools, software and data together with their own to do research (Fig. 1). Wigner Cloud is used as a hardware backend for developing the portal. We are also involved in the development of machine learning methods, like artificial neural networks for inferring antibiotic resistance based on the genetic sequences of bacteria.

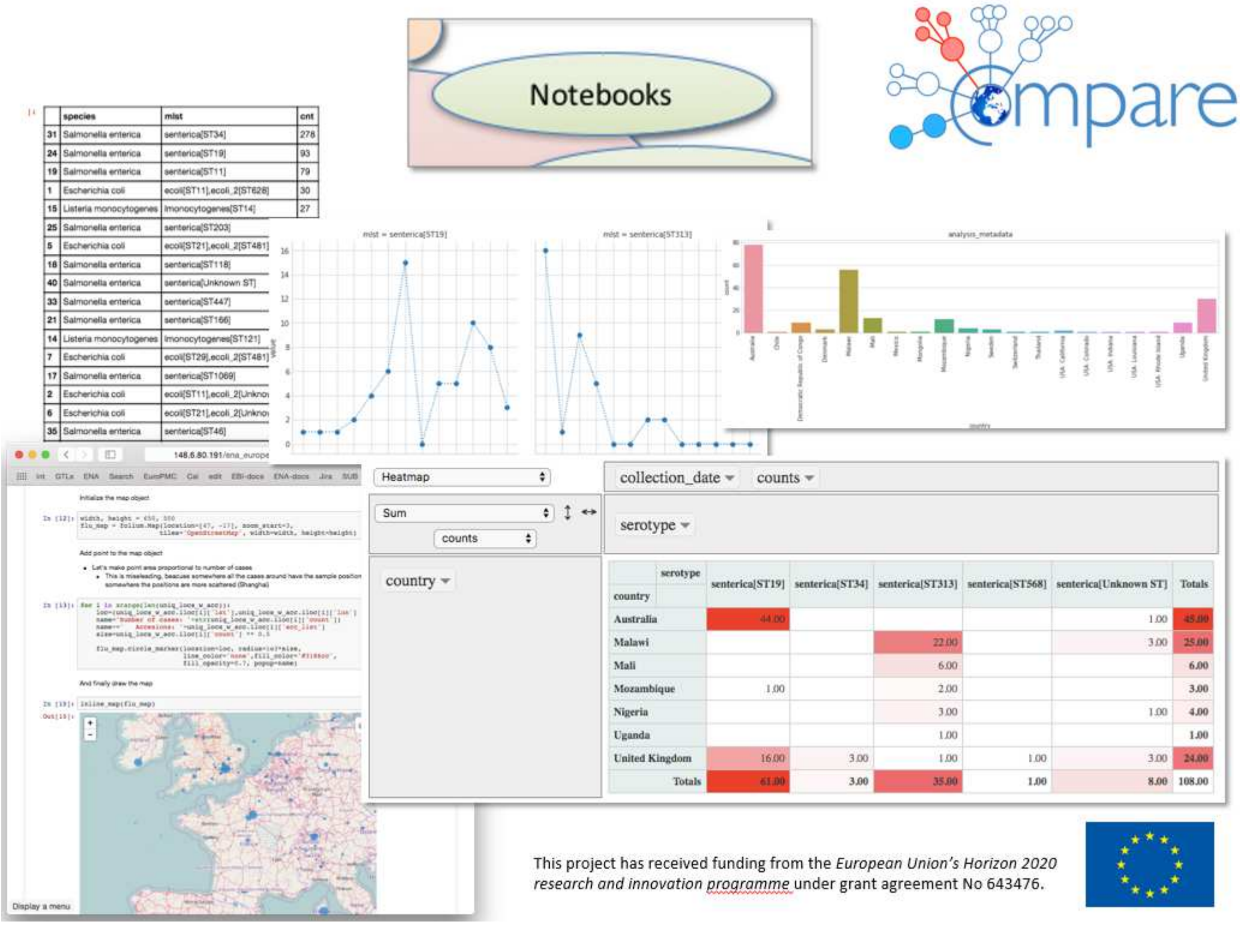


Figure 1. *Snapshot of pathogen genome data analysis in the COMPARE Data Hub.*

Grant

Compare: Horizon 2020 program GA 643476: COllaborative Management Platform for detection and Analyses of (Re-)emerging and foodborne outbreaks in Europe (Node coordinator: I. Csabai, 2014-2019)

International cooperation

Technical University of Denmark National Food Institute (Copenhagen, Denmark) (FM. Aarestrup)

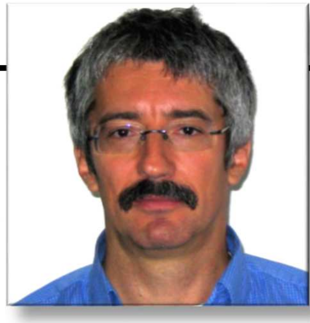
Erasmus Medical Centre Department of Viroscience (Rotterdam, Netherlands) (M. Koopmans)

The European Bioinformatics Institute European Nucleotide Archive (Cambridge Hinxton, United Kingdom) (G. Cochrane)

INSTITUTE FOR
SOLID STATE PHYSICS AND OPTICS*

* **Abbreviations in the researcher lists of the scientific projects:**
#: PhD student
A: associate fellow
E: professor emeritus

S-C. Long-range order in condensed systems



Balázs Újfalussy, Péter Balla[#], Gábor Csire[#], Annamária Kiss, Krisztián Palotás, Karlo Penc, István Tüttő[A], Lajos Károly Varga[A], Ádám Vida[#], Levente Vitos

Multiferroic materials. — During the last few decades, the great potential of multiferroic materials in realizing magnetoelectric memory devices has led to the revival of the magnetoelectric effect and the search for multiferroic compounds. In multiferroics-based memory devices, the writing and reading of magnetic bits by electric field may be realized via the magnetoelectric coupling between the ferromagnetic and ferroelectric orders. However, ferro-ordered phases are extremely sensitive to externals fields. As an alternative approach, information could be stored in antiferromagnetic domains, a concept proposed for metallic compounds in the realm of antiferromagnetic spintronics. We searched whether similar phenomena happen in insulators with coupled antiferromagnetic and antiferroelectric orders. In $LiCoPO_4$ we experimentally demonstrated that the magnetoelectric effect can be exploited not only for the control but also for the identification of antiferromagnetic domains via the strong directional dichroism detected in the THz frequency range -- the absorption coefficients in $LiCoPO_4$ were different for light propagating along and opposite to a given direction in the crystal. Furthermore, we developed a microscopic theory identifying the main microscopic mechanism behind the magnetoeletric effect, which implies that the same effect arises in other antiferromagnets as well. We expect our study will motivate search for multiantiferroic materials. Moreover, the same principle can also be used for the imaging of antiferromagnetic domains with micrometer resolution in these materials via conventional optical absorption measurements.

Superconductivity: We have developed a relativistic spin-polarized microscopic theory for realistic superconducting materials which can treat relativistic effects and superconductivity together with spin and orbital magnetism on the same footing.

As an application, we have studied Nb/Au/Fe heterostructures where long-period oscillations were found in the critical temperature as a function of the gold thickness and no theoretical explanation existed. We placed different number of Au layers between the Nb and Fe layers, where a face-centered cubic (fcc) growth is assumed for the Au overlayers. While the results show that the Au layers remained non-magnetic, spin-polarized bands around the Fermi level can be observed as shown in the Fig. 1. This is the consequence of the different confinement for the spin-up and spin-down electrons: the spin-up electrons are confined in the Au layers only, while the spin-down electrons experience a confinement in both the Au and Fe layers. Therefore, due to the different confinement lengths between the spin channels, more bands are observed for the spin-up states than for the spin-down states. Since the order parameter is influenced mostly by the states in the close vicinity of the Fermi level, we can conclude that a pairing state (in the Au) can occur between two electrons on the induced split parts of the Fermi surface caused by the quantum well states. Hence, the Cooper pair can acquire a finite momentum leading to the oscillation of the order parameter (analogously to the Fulde–Ferrell–Larkin–Ovchinnikov (FFLO) state). In fact, we found an oscillating behavior

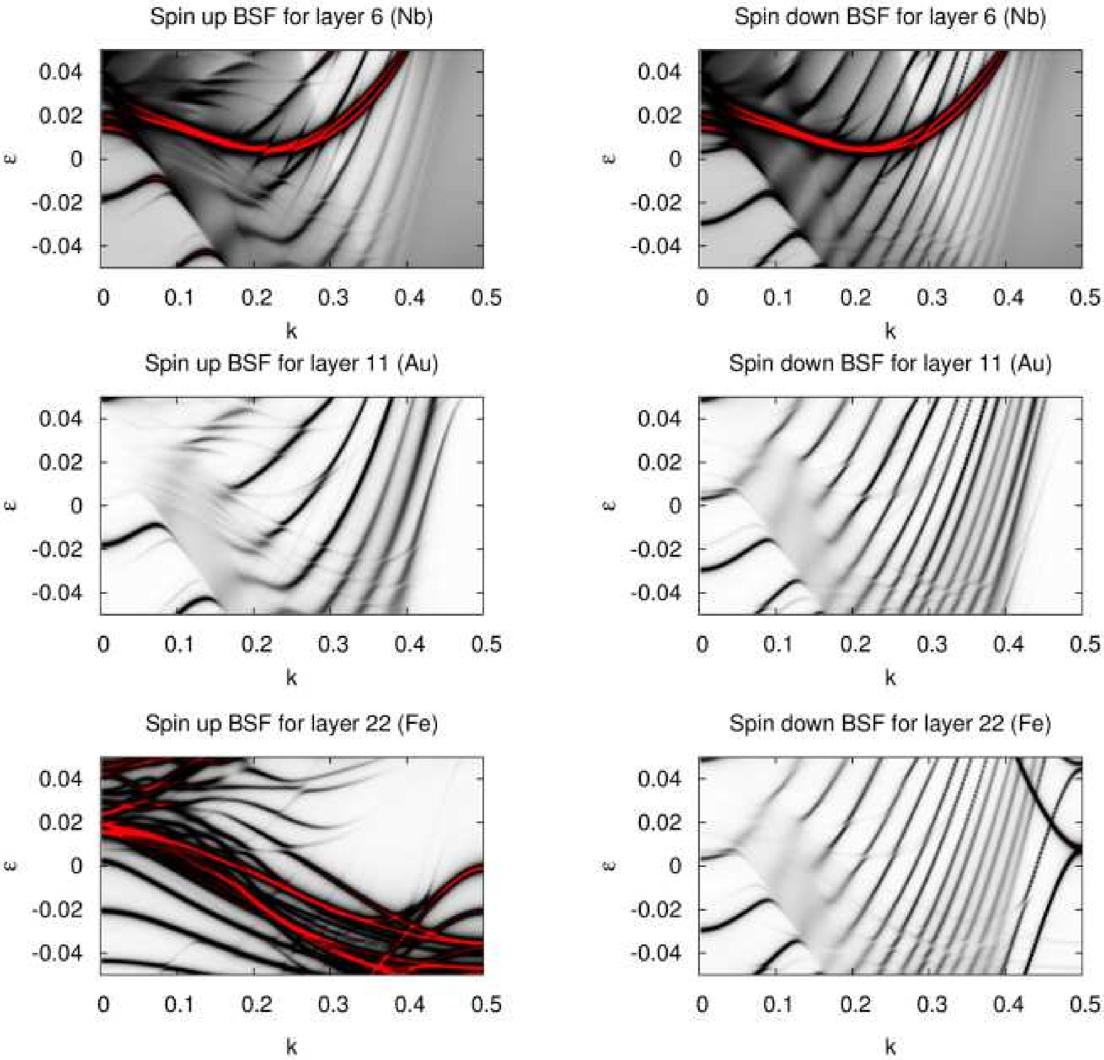


Figure 1. *Quantum well states in Fe/Au/Nb(100). Left column is for ↑ and right column is for ↓ states. First row is for top Nb layer, middle row is for a typical Au and bottom row is for a typical Fe layer.*

of the order parameter as shown in Fig. 2. The period of these oscillations depends on the number of Au overlayers since the band structure and the number of quantum well states depends on the thickness of the Au. For thicker Au overlayers as the number of the quantum well states are increasing, the bands in the spin-up and spin-down channel are separated by smaller and smaller **q** vectors, which leads to an increase of the period of oscillation as a function of the Au thickness. Our theoretical finding explains the oscillating behaviour of the order parameter and suggests that these T_c oscillations observed in that experiment may also be a consequence of the interplay between the quantum-well states and ferromagnetism.

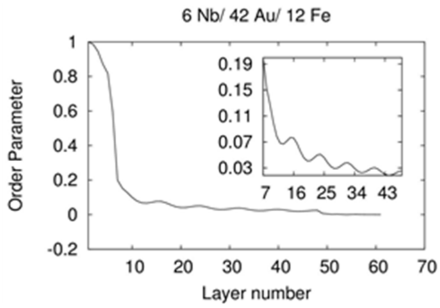


Figure 2. *Oscillation of the order parameter in Fe/Au/Nb(100)*

High-Entropy Alloys. — The investigated multi-component high-entropy alloys (HEAs) represent a solution for an age-old problem: combination of high strength and high ductility of metallic alloys. In this respect, at present two competing materials are in the frontier of materials research:

- Nanoscale particle strengthened steels like the old oxide dispersion strengthened (ODS) alloys and the newly developed co-precipitation strengthened steels and
- Multicomponent high entropy alloys based on solid solution strengthening.

We have followed an integrated computational prediction and experimental validation approach. The computer-aided alloy design was based on first-principles calculations. First, we addressed the forming ability of single-phase HEAs predicting its maximum strength and confirmed the validity of the conjecture about strength (hardness) versus e/a correlation. The theoretical prediction of the elastic properties of various HEAs was contrasted with the available experimental values. Furthermore, we studied the twinning as the fundamental mechanism behind the increased strength and ductility in medium- and high-entropy alloys. Second, we dealt with dual-phase HEAs starting from single-phase NiCoFeCr and adding sp elements like Al, Ga, Ge and Sn. By combining the measured and theoretically predicted temperature-dependent lattice parameters, we revealed the structural and magnetic origin of the observed anomalous thermal expansion behavior. The nanoindentation test revealed a 'fingerprint" of the two-phase structure. The Young's and shear moduli of the investigated HEAs were also determined using ultrasound methods. The correlation between these two moduli suggests a general relationship for metallic alloys.

Grants and international cooperation

OTKA K-115632: Magnetism and superconductivity in intermetallic nanocomposites (B. Újfalussy, 2015-2019) in consortium with BME[3]

OTKA K-106047: Correlated states and excitations in d- and f-electron systems and ultracold Fermi gases (K. Penc, 2013-2017)

NKFIH K-124176: Magnetism, topology, and entanglement in quantum insulators (K. Penc, 2017-2021)

OTKA K-109570: Fundamentals of complex, multi-component metallic alloys (L. Vitos, 2013-2018)

OTKA K128229: Funkcionalizing high entropy alloys for magnetocaloric and thermoelectric applications (L. Vitos, 2018-2022)

OTKA FK-124100 Theoretical study of surfaces of novel materials (K. Palotas, 2017-2021)

HAS NKM-44/2017: Optical magnetoelectric effect and spin dynamics in multiferroics (K. Penc, 2017-2019)

HAS NKM-26/2018 Interaction of electromagnetic radiation with magnetoelectric and magnetic materials (K. Penc, Estonian-Hungarian Joint Research Project)

[3] BME: Budapest University of Technology and Economics

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S-E. Non-equilibrium alloys

Judit Balogh, László Bujdosó, Dénes Kaptás, Tamás Kemény[A], László Ferenc Kiss, Imre Vincze[E]

Magnetic properties of nanoscale Fe-Ag multilayers. — The aim of our work was to give a broad-range map on the variation of the blocking temperature as a function of the Fe-layer (t_{Fe}) and Ag-layer (t_{Ag}) thickness and the number (n) of the bilayers in Fe-Ag granular multilayers. The magnetic relaxation of Fe-Ag multilayers with t_{Fe} in the few monolayers range was first recognized in epitaxial single-crystal multilayers. The relaxation was first attributed to the two-dimensional nature of the ferromagnetic layers but the observation of a linear temperature dependence of the magnetic hyperfine field gave way to explanations based on the island structure of the Fe layers. The deviation of the magnetization of the field-cooled (FC) and zero-field cooled (ZFC) sample undoubtedly indicates a small particle behavior of Fe islands in polycrystalline multilayers. The superparamagnetic properties of such so-called discontinuous or granular multilayers have been the subject of several investigations, similarly to granular alloys prepared by co-deposition. The superparamagnetic properties were shown to be determined by the magnetic anisotropy and the size distribution of the ferromagnetic grains and the strength of the exchange and dipolar interactions between the grains within and between the layers. Our work pointed to the role of the grain-size variation along the subsequent ferromagnetic layers.

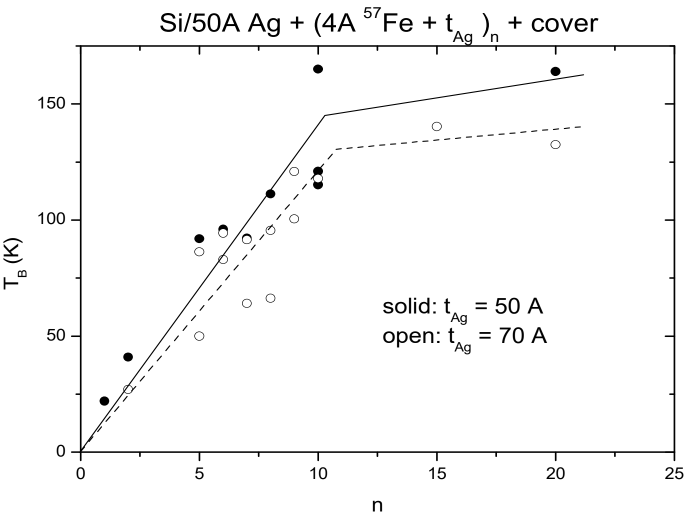

Figure 1. *Blocking temperature (T_B) of (4 Å Fe + t_{Ag})$_n$ multilayers as a function of bilayer number for t_{Ag} = 50 Å (solid symbols) and 70 Å (open symbols). The solid and dashed lines are guides to the eye for the solid and open symbols, respectively.*

The dependence of the blocking temperature (T_B) on the bilayer number is shown in Fig. 1, where solid and open symbols denote two series of samples with t_{Ag} = 50 and 70Å and T_B is measured by the maximum value of the ZFC magnetization curve. It is evident at a first glance that the scatter of the T_B values is significant, which is basically due to the relatively large error of the nominal layer thickness in the few Å layer-thickness range. In spite of the large experimental errors, one can make two definite observations; (i) the blocking temperature increases monotonically with the bilayer number, showing a tendency to

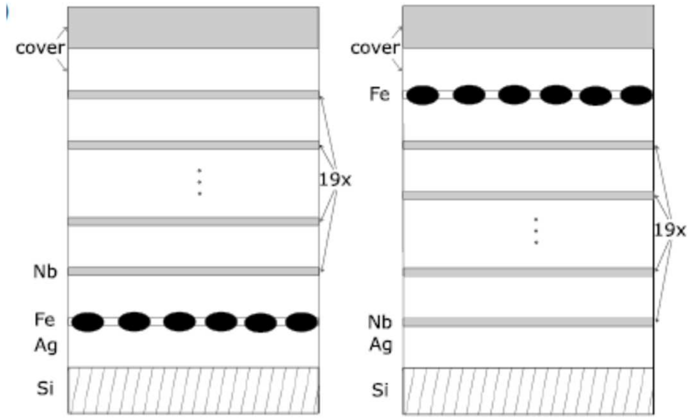

Figure 2. *Schematic view of a special Fe-Ag/Nb-Ag composite multilayer pair with bilayer number of n = 20, containing one Fe layer of 4 Å either in the bottom bilayer (left panel) or in the top bilayer (right panel). The equal thickness of the bottom and top Fe layers was ensured by the simultaneous deposition of the layers.*

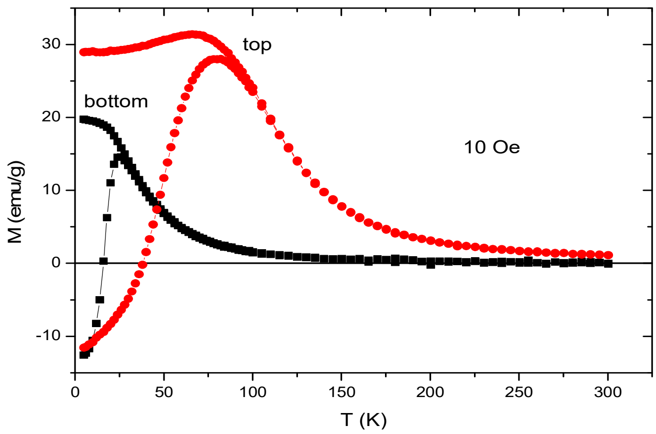

Figure 3. *Magnetization as a function of temperature measured at 10 Oe for the Si/70 Å Ag + 4 Å Fe + (70 Å Ag + 4 Å Nb)$_{19}$ (bottom) and Si/(70 Å Ag + 4 Å Nb)$_{19}$ + 70 Å Ag + 4 Å Fe) (top) multilayer. For each sample, the lower curve (with the maximum) belongs to the ZFC condition while the upper curve to the FC condition.*

saturation and (ii) the t_{Ag}= 70 Å points (open symbols) lie systematically below the t_{Ag}= 50 Å points (closed symbols). Observation (ii) can evidently be explained by the decrease of magnetic interactions between the ferromagnetic layers as the distance between them increases. Dipolar interactions may also contribute to observation (i) as some previous works have already shown in the literature, but the observed changes were smaller.

Another possible cause, namely that the grain size may vary along the multilayer stack, has been demonstrated by our experiment shown in Figs 2 and 3. A composite multilayer pair with bilayer number of *n* = 20 was fabricated which contained only one Fe-Ag bilayer, the rest being composed of non-magnetic Nb-Ag bilayers, as shown in Fig. 2. The multilayer with the Fe layer on the top has a higher blocking temperature (T_B = 80 K) than that with the Fe layer on the bottom (T_B = 25 K), but the increase is smaller than that what can be seen in Fig. 1. These results suggest that the dipolar interactions between the magnetic layers and the grain-size variation along the layer structure might equally play a role in the relation between T_B and the bilayer number. The respective role of these factors should be further studied.

Grants

OTKA K-112811 Magnetic Multilayers Modified by Amorphous Alloys (J. Balogh, 2015-2019)

International cooperation

Department of Physics, Shiga University of Medical Science (Shiga, Japan) (J. Balogh)

Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (Jülich, Germany) (J. Balogh)

Publications

Articles

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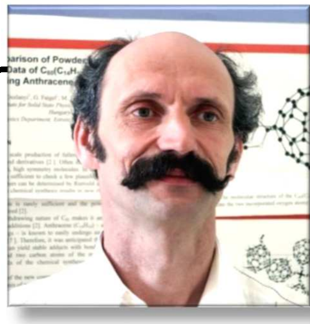
S-F. Laboratory for advanced structural studies



Gyula Faigel, Ferenc Borondics, Gábor Bortel, Dávid Földes[#], László Gránásy, Katalin Kamarás, Bálint Korbuly[#], Éva Kováts, Péter Matus, Katalin Németh[#], Gábor Oszlányi, Áron Pekker, Sándor Pekker, Frigyes Podmaniczky[#], Tamás Pusztai, László Rátkai[#], Hajnalka-Mária Tóháti[#], Gyula Tóth, György Tegze, Miklós Tegze

LASS carries out research in three areas: carbon based materials, computational material science and x-ray related methods. In the last year, we have reached significant results in all of these fields.

Carbon based systems. — As a new category of solids, crystalline materials constructed with amorphous building blocks expand the structure categorization of solids. New amorphous carbon clusters are found by compressing C_8H_8/C_{60} cocrystals, in which the highly energetic cubane (C_8H_8) exhibits unusual role. The significant role of C_8H_8 is to stabilize the boundary interactions of the highly compressed or collapsed C_{60} clusters, which preserve their long-range ordered arrangement up to 45 GPa. With increasing time and pressure, the gradual random bonding between C_8H_8 and carbon clusters, -due to "energy release" of highly compressed cubane, leads to the loss of the ability of C_8H_8 to stabilize the carbon cluster arrangement. Thus, a transition from short-range disorder to long-range disorder (amorphization) occurs. The spontaneous bonding reconstruction most likely results in a 3D network in the material, which can create ring cracks on diamond anvils.

Computational material science. — During biomineralization, such as during the formation of bones, teeth, or mollusc shells and coral skeletons, hierarchically structured organic-inorganic composites of unique properties form, where the unique properties originate from their microstructure. We used traditional computational materials science tools to model the formation of these complex microstructures. In collaboration with German experimental scientists, we have reported a spectacular agreement between the microstructure of mollusc shells determined by experimental methods (including electron microscopy, electron back-scattering diffraction (EBSD), and X-ray micro-tomography) and the microstructure predicted by the phase-field theory. Such a complex structure was addressed for the first time by phase-field modelling, which may open the way for the modelling of even more complex biomineralization processes.

X-ray related methods. — Our research concentrated on X-ray free-electron laser (XFEL) related experiments. We took part in a holographic experiment on free-flying nanoparticles. We showed that structural information of individual nanoparticles could be obtained using a single XFEL pulse only.

Further, we gave general guidelines for the treatment of experimental data from coherent diffractive imaging and incorporated particle symmetry into the orientation determination in single-particle imaging (Fig. 1).

[#] Ph.D student

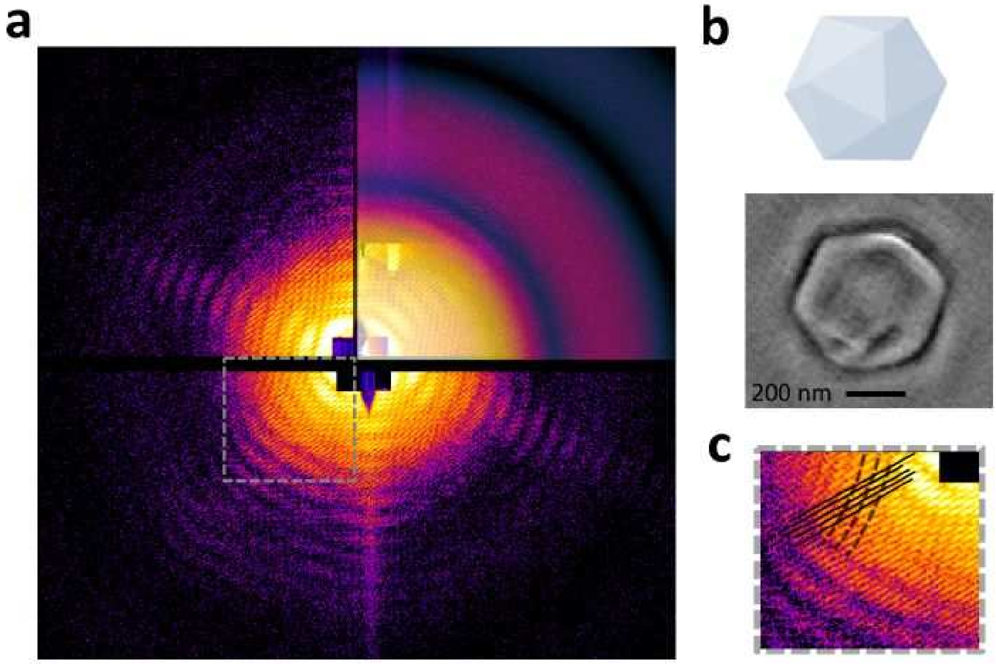


Figure 1. *(a) X-ray diffraction pattern of 3 particles, 2 Ar clusters and a Mimi virus. The diffraction pattern can be analogously analized as a hologram. (b) The icosahedral envelop of the mimi virus and its 2D SEM projection. (c) Enlarged part of (a) showing two fine line patterns, corresponding to the 3 particles in the beam.*

Grants

OTKA K-115504. Structure determination of biological particles with x-ray free electron laser (M. Tegze 2015- 2019).

NKFIH K-115959, Pattern formation in far-from equilibrium systems (L. Gránásy, 2016–2019).

NKFIH SNN-118012 Correlated electrons in confined molecular systems (K. Kamarás 2016-2019)

NKFIH PD-121320 Spectroscopic study of low-dimensional materials (Á. Pekker 2016-2019)

NKFIH FK-125063 Spectroscopic study of chemically modified low-dimensional materials (Á. Pekker 2017-2021)

NKFIH NN-127069 Pb-free perovskite solar cells with long-term stability (K. Kamarás 2018-2020)

VEKOP-2.3.3-15-2016-00001 Determination of atomic structure of nanosystems (K. Kamarás 2016-2018)

VEKOP-2.3.2-16-2016-00011 Strategic workshop for the technological challenges of renewable energy systems (K. Kamarás 2017-2020)

OTKA-KKP-126749 (L. Gránásy 2018-2022)

OTKA-NN-125832 (T. Pusztai 2018-2021)

International cooperations

Institut de Physique de la Matière Complexe, EPFL, Lausanne, Switzerland, Prof. László Forró, 1 joint publication

Department of Mechanical Engineering, University of Tokyo, Prof. Shigeo Maruyama, 1 joint publication

Cardiff University, School of Chemistry, Cardiff, United Kingdom, Prof. D. Bonifazi, 1 joint publication

State Key Laboratory of Superhard Materials, College of Physics, Jilin University, , Changchun, 130012 China, 1 joint publication

Physique de la Matière Condensée, École Polytechnique, CNRS, 91128 Palaiseau, France, Dr. Hervé Henry, 1 joint publication

Center for Molecular Bioengineering Technische Universität Dresden, Germany, 1 joint publication

EDAX, Tilburg, The Netherlands, 1 joint publication

ESRF, Grenoble, France 2 joint publications

LCLS, Stanford, USA 2 joint publications

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Articles

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See also: S-D.2, S-Q.1

S-G. Radiofrequency spectroscopy

György Kriza, Mónika Bokor, Kálmán Tompa[E]

Melting diagram of protein solutions and its thermodynamic interpretation — NMR characteristics of frozen aqueous solutions provide direct information on the immobile and partially or fully mobile parts of the molecules. The purpose is the thermodynamic characterization of protein systems. The studies were focused on the proteins ubiquitin (UBQ) and early response to dehydration 10 (ERD10). These proteins are representatives of distinct structural classes, UBQ is a globular protein and ERD10 is intrinsically disordered protein (IDP). The melting diagrams (*MD*s) of the protein solutions are the amount of the mobile hydration water as a function of temperature or potential barrier for this motion (Fig. 1). The amount of mobile hydration water is measured by the amplitude of the slowly decaying ^{1}H NMR signal component expressed as a fraction of the total water amount. Temperature is measured as normalized functional temperature T_{fn} = T/273.15 K (T is absolute temperature) and the potential barrier for the motion of water is E_a = T_{fn}·6.01 kJ/mol, where T_{fn} is multiplied with the heat of fusion of water. Hydration is grams water/grams protein.

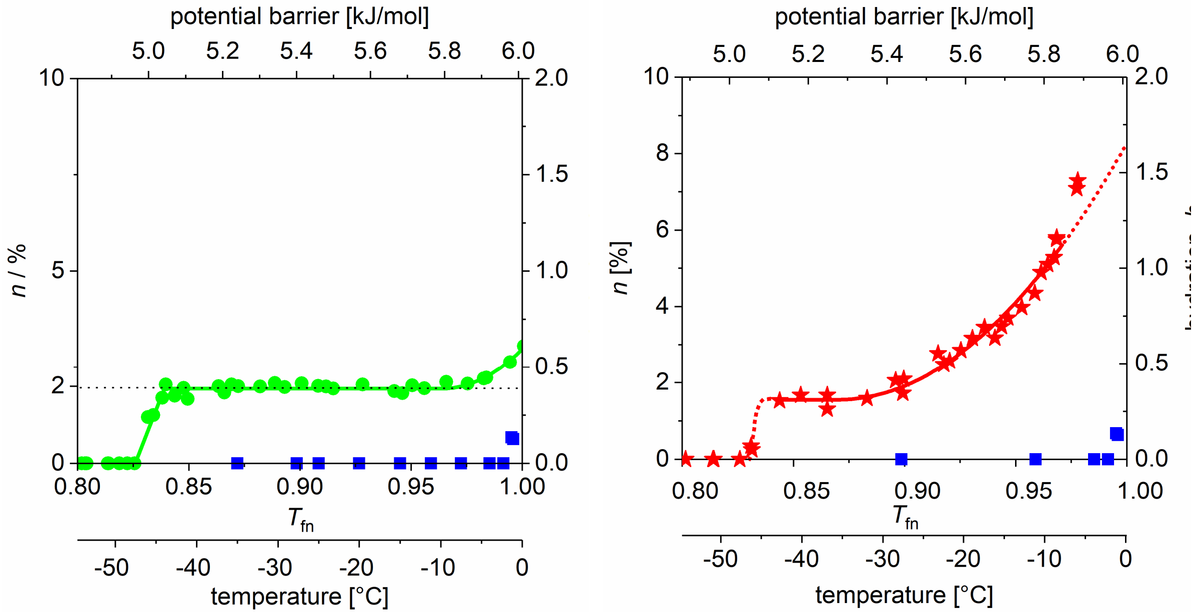

Figure 1. *Melting diagram of proteins ubiquitin (UBQ, green circles) and early response to dehydration 10 (ERD 10, red stars), both dissolved in water (50 mg/mL) and that of frozen water under identical conditions (blue squares).*

In aqueous solutions, melting (*i.e.* beginning of molecular motion) of protein-bound water begins at a much lower temperature than the melting of bulk ice. Each protein has a unique *MD* that results from its individual thermodynamic characteristics. The *MD* of globular and ID

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proteins vastly differ. They can be characterized by temperature-independent sections (globular proteins) or without them (IDPs) or can have a small such section (partly IDP).

For UBQ, at melting (-46 °C), the steep step shows that there are water molecules in the first hydrate shell that are bound almost identically, so the relevant molecular surface is equipotential. The potential field of nearly identical elements resembles the feature of hydrogen bridges. The next wide region is a plateau, in this excitation energy region no new water molecules begin to move, because there are no water molecules that are bound by corresponding energy to the protein. The hydrogen bridges here link the bulk of the molecule to a globule. The water molecules, which are bound to surface areas more accessible to water, begin to move at higher potential barriers. For ERD10, the melting occurs at higher temperature (-42 °C) what it is common in IDPs. The plateau after the melting step is significantly narrower than that observed in globular proteins. Then, a phase of continuous rise in *MD* is observed indicating that a much larger part of the protein surface is accessible to water in ERD10, in an IDP, than in globular proteins. This means that the solvent-accessible surface of ERD10 is highly heterogeneous energetically which is characteristic to IDPs.

Grants

Research contract with the HAS, Research Centre for Natural Sciences, Institute of Enzimology

International cooperation

VIB Structural Biology Research Center (SBRC), Vrije Uneversitaet, Brussel, Belgium

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S-I. Electrodeposited nanostructures

László Péter, Imre Bakonyi[E], Vandri Ahmad Isnaini[#], Lajos Pogány[A], Sándor Zsurzsa[#]

Component distribution of electrodeposited alloys. — Electrodeposited alloys prepared with constant current density exhibit a unique near-substrate component distribution. The preferentially deposited metals accumulate near the substrate, and the decay of the initial zone of uneven composition is 150-200 nm thick regardless of the alloy constituents. This effect has a great importance in the deposition of nanostructures in which the total layer thickness is often less than the decay length scale of the spontaneous composition variation. It was shown that two countermeasures can provide deposits with even composition also in the near-substrate zone: a, application of pulse plating, and b, the application of uniform convection conditions. The results related to many deposit compositions were summarized in a comprehensive review article.

Special attention was devoted to the composition depth profile of Fe-Co-Ni deposits. It was shown that the composition variation as measured with either sputtering-based depth profiling methods or cross-sectional scans in a transmission electron microscope (TEM) are essentially identical. The advantage of the application of the TEM was that the length scale of the composition variation and that of the change in the crystallographic properties (grain size and orientation) could be seen for identical samples. It was revealed that variations in the composition and in the crystallographic properties are independent of each other. (This work was performed in co-operation with the Josef Stefan Institute, Ljubljana, Slovenia.)

Structural properties of electrodeposited metals. — The structural properties of electrodeposited nanocrystalline Ni films were analyzed with TEM and X-ray line profile analysis (XLPA). The effect of saccharin as organic additive on the microstructure, texture and hardness was studied. The addition of the saccharin to the plating baths eliminated the texture and yielded very fine microstructures with high dislocation densities and twin fault probabilities for all solution types tested. A strong correlation was found between the defect density and the grain size.

A plating bath based on nickel sulfate and sodium citrate was developed for the deposition of crack-free Ni–Mo alloy layers of $d > 20$ μm thickness with varying Mo content up to 6 mol%. The increase in the Mo content resulted in a larger dislocation density and twin fault probability as well as a smaller grain size. The presence of saccharin as additive in the bath and the incorporated sulfur content due to the saccharin decomposition led to a further decrease in the grain size. The Mo content of the alloy improved the thermal stability of the alloys, while the sulfur incorporation had an adverse effect. The sulfur-free $Ni_{94}Mo_6$ alloy

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conserved its nanocrystalline nature with < 50 nm grain size up to 800 K, even though the twin faults and the dislocations annihilate under this annealing condition.

(All works related to the structural studies were performed in co-operation with the Eötvös University and the Centre for Energy Research of the Hungarian Academy of Sciences.)

Industry-oriented research activities. — Electrodeposition has long been playing a vital role in surface finishing by being able to produce a variety of metallic coatings on product surfaces for protective, decorative and various other functional purposes. At a certain level of technological development, there was an increasing demand for coatings with improved deposit performance. This need was the driving force behind the elaboration of new electrodeposition methods, which enable the preparation of coatings with their composition varying along the thickness. Such “compositionally graded coatings” can be classified as compositionally modulated alloys (CMA) or multilayers. In the case of a CMA coating, the alloy deposit composition is continuously modulated along the thickness. In the case of a multilayer coating, the deposit consists of an alternating sequence of two layers with different chemical compositions whereby the constituent individual layers can have a thickness even down to the nanometer scale (for metallic materials, 1 nm corresponds to roughly 4-5 monatomic layers). In collaboration with the Hirtenberger Engineered Surfaces (HES), Austria, we have provided an overview of the development of various pulse-plating methods for the preparation of compositionally graded coatings from a single bath. As a particular case, the historical development of corrosion-protective electrodeposited multilayers based on the Zn-Fe system and their state of the art was exemplified. This overview was presented at the last European Pulse Plating Seminar in Vienna, organized biannually by HES and was published as a review paper in one of the leading journal of industrial surface finishing.

Calculations taking into account various chemical equilibra (acid-base, complex formation and partition between phases) were performed in order to establish a technique combining dual-phase potentiometric lipophilicity measurement with the partition coefficient method. With a negligible simplification, a linear equation was obtained for calculating both the acid dissociation and the complex formation constants. The method developed proved to be suitable for testing the lipophilicity of drug candidates by using smaller quantities and much less expensive instrumentation than conventional techniques. The complex-formation constants obtained for all drug candidate compounds tested reproduced very well the values reported by using other methods. (This work was performed in co-operation with the following partners: Compound Profiling Laboratory of the Gedeon Richter Plc., Budapest University of Technology and Economics and Cyclolab Cyclodextrin Research and Development Ltd.)

Grant

Research Cooperation Project “Periodic magnetic nanostructures by electrochemical approaches: a novel route towards the fabrication of magnonic crystals” supported by the Humboldt Foundation Research Group Linkage Programme between the Wigner RCP and the Leibniz Institute IFW-Dresden (Hungarian project leader: I. Bakonyi, 2017-2019)

International cooperation

COST Action MP1407 (17 COST and 3 non-COST countries): Electrochemical processing methodologies and corrosion protection for device and systems miniaturization: e-MINDS (Management Committee members: I. Bakonyi and L. Péter, 2015-2019)

MTA NKM-8/2018 (Hungarian-Bulgarian bilateral academic exchange project): Magnetic alloys and multilayers prepared by oscillating electrochemical reactions (Hungarian project leader: L. Péter, 2016-2018)

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S-K. Liquid structure

Pál Jóvári, László Kőszegi[A], Ildikó Pethes, Szilvia Pothoczki, László Pusztai, Erzsébet Sváb[A], László Temleitner

Understanding disordered structures. — Our research group is involved in the investigation of short range order of liquids, amorphous materials and disordered crystals. We combine experimental data, such as X-ray and neutron diffraction structure factors and EXAFS spectra, with computer modeling tools, such as Reverse Monte Carlo (RMC) and molecular dynamics (MD) simulations. As a result of such a modelling approach, large configurations (typically tens of thousands of atoms) are provided that are energetically reasonable and consistent (within errors) with experimental data. These configurations are then subjected to various geometrical analyses, so that specific questions concerning the structure of a material may be answered. The group is also responsible for the maintenance and operation of the MTEST neutron diffractometer installed at the 10 MW Budapest Research Reactor. Below we provide some selected results from the year 2018.

Covalent glasses. — Short-range order of $As_{40-x}Cu_xTe_{60}$ (x = 0, 10, 20, 25, 30) glasses has been studied by neutron- and X-ray diffraction, combined with extended X-ray absorption fine structure (EXAFS) measurements at the K-edges of all components. Large-scale structural models have been generated by fitting the experimental datasets simultaneously in the framework of the reverse Monte Carlo simulation technique. These simulations revealed that there are about 3 As or Te atoms around As and 2 As or Te atoms around Te. Both As and Te possess Cu neighbors.

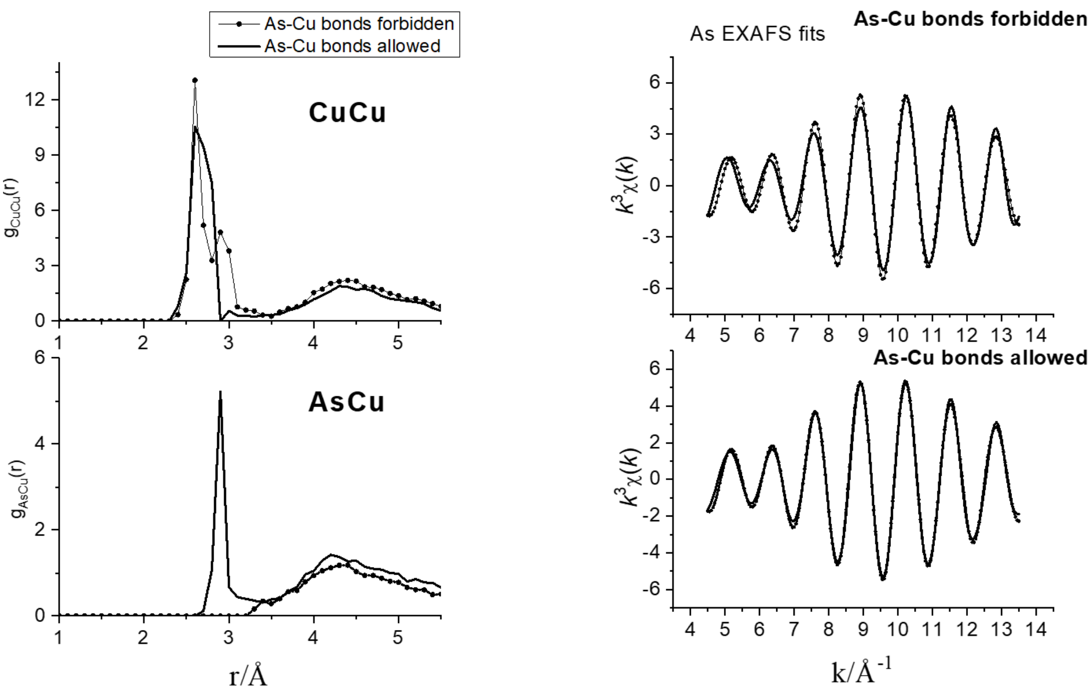

Figure 1. *Comparison of As-Cu and Cu-Cu partial pair correlation functions (left) and As K-edge EXAFS fits (right) of glassy $As_{20}Cu_{20}Te_{60}$ obtained with and without As-Cu bonds*

The presence of Cu-As bonds was proven by dedicated simulation runs. In Fig. 1, we compare the Cu-Cu and Cu-As partial pair correlation functions and the $As_{20}Cu_{20}Te_{60}$ As K-edge fits obtained with and without Cu-As bonds. Two observations can be made here: *i*) the fit quality worsens upon eliminating Cu-As bonding, *ii*) a secondary Cu-Cu peak appears in the Cu-Cu partial pair correlation function to compensate for the lack of the Cu-As peak. This secondary Cu-Cu peak is necessary to maintain at least the Cu K-edge EXAFS fit quality. The presence of As-Cu bonds was verified by dedicated simulation runs. The Cu-Te bond length is 2.57±0.02Å while the Cu-As distance is as high as 2.86±0.04Å. The results further showed that besides As and Te, Cu atoms also bind to Cu. The total coordination number of Cu is significantly higher than 4 for x = 25 and 30.

Temperature-dependent structure and dynamics of ethanol-water mixtures at low alcohol contents. — By making use of literature X-ray diffraction data, extensive molecular dynamics computer simulations have been conducted for ethanol-water liquid mixtures in the water-rich side of the composition range, with 10, 20 and 30 mol% of the alcohol, at temperatures between room temperature and the experimental freezing point of the given mixture. All-atom type (OPLS) interatomic potentials have been assumed for ethanol, in combination with two kinds of rigid water models (SPC/E and TIP4P/2005). Both combinations have provided excellent reproductions of the experimental X-ray total structure factors at each temperature; this provided a strong basis for further structural analyses. Beyond partial radial distribution functions, various descriptors of hydrogen-bonded assemblies, as well as of the hydrogen-bonded network have been determined from the simulated particle configurations. A clear tendency was observed towards that an increasing proportion of water molecules participate in hydrogen bonding with exactly 2 donor and 2 acceptor sites as the temperature decreases. Concerning larger assemblies held together by hydrogen bonding, the main focus was put on the properties of cyclic entities: it was found that, similarly to methanol-water mixtures, the number of hydrogen-bonded rings has increased with decreasing temperature. However, for ethanol-water mixtures the dominance of not the six-, but of the five-fold rings could be observed (see Fig. 2).

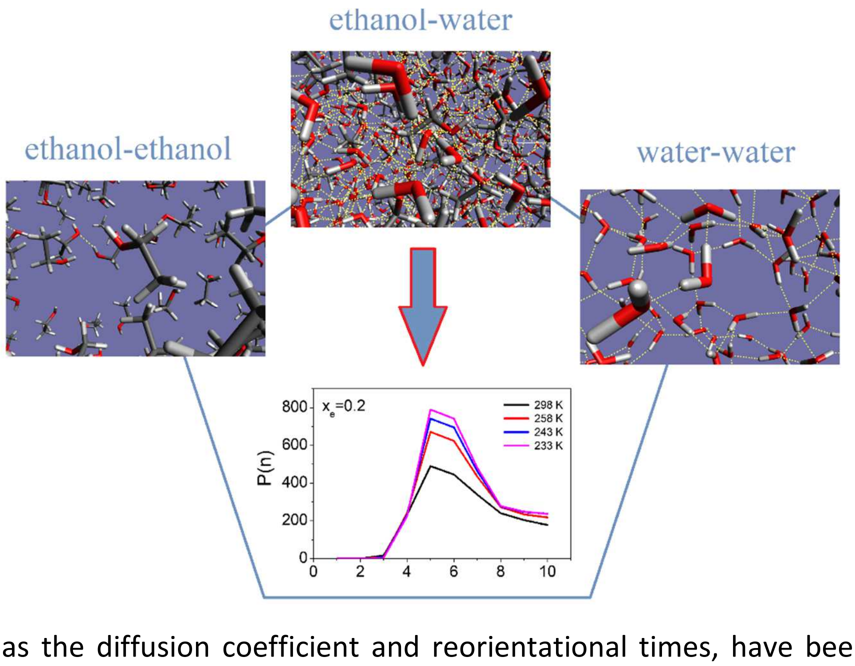

Figure 2. *Temperature dependence of hydrogen bond ring size distribution in water-20 mol% ethanol mixture*

Starting from the molecular dynamics simulations mentioned above, we took a closer look at the time-dependent behavior of molecules. Temperature-dependent hydrogen bond energetics and dynamical features, such as the diffusion coefficient and reorientational times, have been determined for ethanol-water mixtures with 10, 20 and 30 mol % of ethanol. Concerning pairwise interaction energies between molecules, it was found that water-water interactions become stronger, while ethanol-ethanol ones become significantly weaker in the mixtures, than the corresponding values characteristic to the pure substances. Concerning the diffusion processes, for all concentrations the activation barrier of water and ethanol molecule becomes very similar to each other. Reorientational motions of water and ethanol become slower as ethanol concentration is increasing. Characteristic reorientational times of water in the mixtures are substantially longer than these values in the pure substance. On the other hand, for ethanol this change is only moderate. Reorientational motions of water (especially the ones related to the H-bonded interaction) become very similar for those of ethanol in the mixtures.

The structure of the simplest liquid aldehydes. — Although aliphatic aldehydes (a.k.a. alkanals, compounds with chain-end –CHO groups) constitute an essential group of organic substances, structural studies of them are scarce. Synchrotron X-ray diffraction experiments and molecular dynamics simulations have been performed on simple aliphatic aldehydes in the liquid state, from propanal to nonanal. The performance of the OPLS all-atom interaction potential model for aldehydes has been assessed via direct comparison of simulated and experimental total scattering structure factors. In general, MD results reproduce the experimental data at least semi-quantitatively. However, a slight mismatch can be observed between the two datasets in terms of the position of the main diffraction maxima. Partial radial distribution functions (PRDF) have also been calculated from the simulation results. Clear differences could be detected between the various O-H partial radial distribution functions, depending on whether the H atom is attached to the carbon atom that is doubly bonded to the oxygen atom of the aldehyde group or not. Based on the 3 different O-H PRDF-s, as well as on the various H-H PRDF-s, it may be suggested that neighboring molecules turn toward each other (somewhat) preferentially by their aldehyde ends. From $g_{OO}(r)$ and $g_{C'C'}(r)$, and from intermolecular angular correlations it may be discerned that no (or at most, extremely weak) orientational correlations are present between neighboring aldehyde groups.

As a follow-up of the above series of experiments, the total scattering structure factors of pure liquid *n*-pentanol, pentanal, and 5 of their mixtures have been determined by high-energy synchrotron X-ray diffraction experiments. For the interpretation of the measured data, molecular dynamics computer simulations were performed, utilizing 'all-atom' type force fields. The diffraction signals, in general, resemble each other over most of the monitored scattering variable (*Q)* range above 1 $Å^{-1}$, but the absolute values of the intensities of the small-angle scattering maximum ('pre-peak', 'first sharp diffraction peak') around 0.6 $Å^{-1}$ change in an unexpected fashion, non-linearly with the composition. MD simulations are not able to reproduce this low-*Q* behavior; on the other hand, they do reproduce the experimental diffraction data above 1 $Å^{-1}$ rather accurately. Partial radial distribution functions are calculated based on the atomic coordinates in the simulated configurations. Inspection of the various O-O and O-H partial radial distribution functions clearly shows that both the alcoholic and the aldehydic oxygens form hydrogen bonds with the hydrogen atoms of the alcoholic OH-group.

Aqueous salt solutions. —Highly concentrated aqueous lithium chloride solutions have been investigated by classical molecular dynamics (MD) and reverse Monte Carlo (RMC) simulations. At first, MD calculations have been carried out by applying twenty-nine combinations of ion-water interaction models at four salt concentrations. The structural predictions of the different models have been compared, the contributions of different structural motifs to the partial pair correlation functions (PPCF) have been determined. Particle configurations obtained from MD simulations have been further refined using the RMC method to get better agreement with experimental X-ray and neutron diffraction data. The PPCFs calculated from MD simulations have been fitted together with the experimental structure factors to construct structural models that are as consistent as possible with both the experimental results and the results of the MD simulations. The MD models have been validated according to the quality of the fits. Although none of the tested MD models can describe the structure perfectly at the highest investigated concentration, their comparison made it possible to determine the main structural properties of that solution as well. It was found that four nearest neighbors (oxygen atoms and chloride ions together) are around a lithium ion at each concentration while in the surroundings of the chloride ion, hydrogen atom pairs are replaced by one lithium ion as the concentration increases. While in pure liquid water four water molecules can be found around a central water molecule, near the solubility limit nearly all water molecules are connected to two chloride ions (via their hydrogen atoms) and one lithium ion (by their oxygen atoms).

Grants

OTKA SNN-116198: Structure and thermodynamics of Hydrogen bonded liquids (L. Pusztai, 2016-2019)

NKFIH K-124885: Investigation of electrolyte solutions by theoretical and experimental methods (I. Bakó, NSRC HAS; Wigner-responsible: L. Pusztai, 2017-2021)

NKFIH KH 130425 : The influence of pressure and temperature on the structure of alcohol-water mixtures (L. Pusztai, 2018-2020)

NKFIH-FK 128656: Structural study of hydroxy-containing compounds in aqueous solutions (Sz. Pothoczki, 2018-2022)

NKFIH-JIST: Diffraction and computer simulation studies of structural disorder (L. Temleitner, 2017-2018)

HAS-LAS Hungarian-Latvian bilateral: X-ray Absorption Experiments for Disordered and Nanocrystalline systems: Interpereting Data via Reverse Monte Carlo Methods (L. Pusztai, 2016-2018)

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S-L. Nanostructure research by neutron scattering

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The research group has been involved in several research projects and various user measurements performed at the neutron scattering instruments operated by the members of the Group: Small-Angle Neutron Scattering instrument, Time-of-Flight spectrometer, Three-axis spectrometer, Reflectometer and PSD Diffractometer. Some of the results are specified below.

A novel approach in the mineralogy of Carpathian mahogany obsidian using complementary methods. — The study of Carpathian obsidians has been performed with the aid of a multidisciplinary approach. Carpathian obsidians have various macroscopic features. They are typically black or grey and their transparency ranges from clear to opaque. The Tolcsva source, very rarely, can yield brown or red ('mahogany' type) obsidian. In 2007, the exact location of the red variant's outcrop was identified on the Szokolya hill (Tolcsva). In order to understand the possible reasons for the colouring of red obsidian, a multiple-method approach has been used for the analysis of the samples. For comparison, other Carpathian type, namely black obsidian from Tolcsva, and a red obsidian from Bogazkoy (Anatolia) were also studied. The measurements were carried out in collaboration with groups of the Centre for Energy Research of HAS and the Hungarian National Museum. Prompt gamma activation analysis (PGAA) measurements were done to determine the bulk elemental composition. Mössbauer spectroscopy and transmission electron microscopy (TEM) were used to identify the presence of ferrous or ferric iron. We used small-angle neutron scattering (SANS) for characterization of the nanostructure, measuring their anisotropy and surface or volume fractal dimensions. Black obsidians showed isotropy, while mahogany samples displayed a considerable anisotropy in the bulk pore orientation (Fig. 1). According to our results, a large amount of the iron is dominantly located in different phases in the case of mahogany and black obsidians. The differences between the red and black variants could be also explained by the different oxidation states of the Fe-ions, which may explain the colour difference.

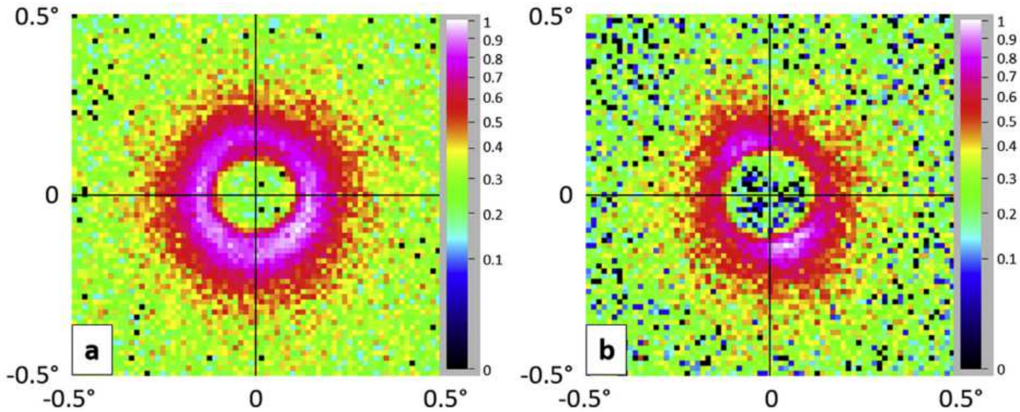

Figure 1. *2D scattering pattern of Tolcsva mahogany (a) and Bogazkoy mahogany (b) samples, measured on the time-of-flight small-angle neutron scattering (FSANS) instrument.*

Study on polyester-carbon nanotube–graphite composites by small-angle neutron scattering. — Polymer nanocomposites prepared by carbon nanotube (CNT) addition were first reported in the 1990's. Since then, a great number of scientific papers have been published on this topic. However, the great differences between the CNTs produced by different companies, the aggregation and surface characteristics of the CNT fillers, the amount of impurities and defects makes the comparison of the results difficult. The fractal dimension of fracture surfaces or of the bulk volume of prepared nanocomposites is linked to the strength, thermal and electrical conduction properties etc. of them. The studies carried out now and the description of physical characteristics of the polymer composites lead to a better understanding of the relation between the nano- and macro-characteristics, and to a more relevant comparison of the composites prepared by different laboratories and companies.

Samples with various multiwalled CNT and graphite additives were prepared in collaboration with a research group from Morocco, with the aid of a clean, economical and environmental friendly method. Small-angle neutron scattering experiments on the samples were carried out at Yellow Submarine and FSANS instruments located at the Budapest Research Reactor. Nanostructural characteristics of the prepared ternary composites (such as the size distribution and agglomeration of the additives, and their fractal characteristics) were determined, that contributed to a better understanding of macroscopical characteristics of these composites.

Synthesis and characterization of a polyurethane carrier used for a prolonged transmembrane transfer of a chili pepper extract. — Red chili peppers have been highly valued in gastronomy and traditional medicine since ancient times. In collaboration with the University of Medicine and Pharmacy, Timisoara, a complex study on the characterization of a new carrier used for encapsulated extract has been performed.

Chili pepper extract was obtained and was physically entrapped inside polyurethane microparticles in order to diminish the irritative potential of this extract. The particle morphology was evaluated by various methods, among them small-angle neutron scattering and scanning electron microscopy (SEM) were performed by our group. SEM images indicated no difference between the capsaicin-loaded and capsaicin-free samples; in both cases the formation of 50–100 µm clusters was visible (Fig. 2), and SANS indicated no differences in the nanometer scale either.

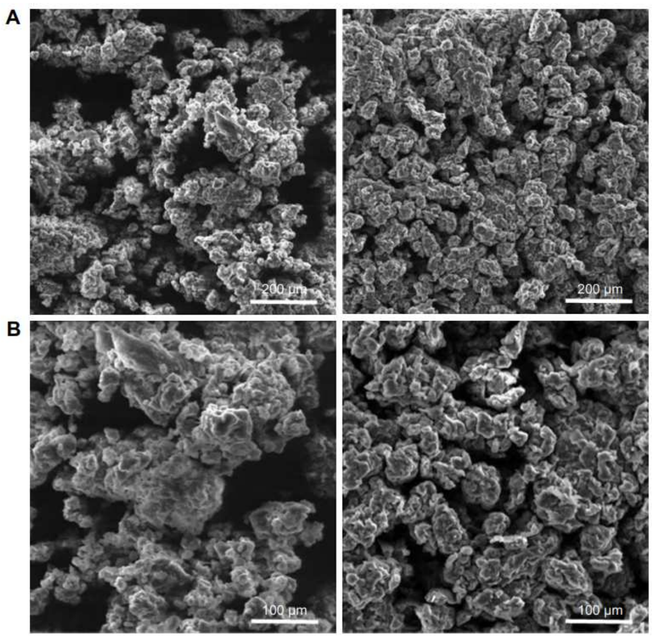

Figure 2. *SEM images of capsaicin-loaded (right) and capsaicin-free (left) samples.*

The encapsulation efficacy and the drug release profile were assessed by UV-Vis spectroscopy. Bioevaluations on mice skin were performed to predict the irritative potential of the samples. The encapsulation of a chili pepper extract inside polyurethane microparticles lead to a non-irritative product with a prolonged release: ~30% of encapsulated extract is released within the first 8 days and a maximum 45% is reached in 2 weeks.

Mesoporous silica materials for different applications. — Various types of templated silica materials have been synthesized and studied by small-angle neutron and X-ray scattering methods. Functionalization of the pore surfaces has been achieved using simple co-condensation of two precursors, with variation of the reaction conditions, or in multistep method by subsequent treatment of the templated porous silica by organic precursors. The method of preparation and the type of additives determine the performance of the materials in different applications. Sorption studies of guest molecules and heavy metals have been performed and the performance of the materials have been optimized for achieving maximal adsorbance, and for the control of the release rate of drug molecules.

Silica based aerogels hybridized with biomolecules (proteins or polysaccharides) are also promising platforms for drug delivery applications. The composition, the pore structure and the hydrophobicity of the biopolymer aerogel predetermine the main properties, each fundamental in drug delivery applications. These properties will determine the release profile (desorption kinetics) of the drugs from the delivery system. By understanding the key factors, which connect the structure to the application, a systematic approach has been developed in designing and fine-tuning hybrid aerogel based drug delivery systems. SANS measurements monitored the deformation and the hydration of the aerogel structure upon interaction with water. In order to visualize the silica matrix and the gelatin phase, the samples were measured in various H_2O/D_2O concentrations in order to match the silica or the gelatin content. The measurements on half and fully saturated samples proved that the hydration of the samples did not affect the silica skeleton and the pore structure.

Structural characterization of chalcogenide systems. — Neutron- and X-ray diffraction techniques were used to study the glassy atomic structure and Reverse Monte Carlo simulations were applied to model the 3-dimensional atomic configurations and thorough mapping of the atomic parameters of the 3-component Ge-Sb-Se and 4-component As-Se-Sb-Te chalcogenides. We determined the short-range order of the amorphous Ge-Sb-Se system. From diffraction measurements it was revealed that the short-range order is formed by the fulfillment of the 8-N rule (germanium has 4, antimony has 3 and selenium has 2 neighbors) and the presence of the chemical order (germanium and antimony bonds primarily to the selenium atom). We found that in the case of the As-Se-Sb-Te system, the 8-N rule is not fulfilled for all atoms. The As and Sb atoms have three neighbors connected to the mixed Te and Se atoms. The glassy network builds up from pyramid units, connected through 2-coordinated Se and Te atoms.

Interfacial roughness correlation in multilayers. – Interface roughness and correlation properties of magnetron sputtered Ni-Ti multilayers were investigated by off-specular x-ray and neutron scattering. GISAS (Grazing Incidence Small-Angle Scattering) measurements were performed in order to complement our reflectometry results. The aim of the experiments was to check whether the interface roughness auto- and cross-correlation can be described by the in-plane and out-of-plane correlation lengths and Hurst-exponent. In the case of X-ray GISAS on periodic samples, we had to modify the linear approximation in the frames of the Distorted-Wave Born Approximation for large scattering angles and roughness.

Taking into account the non-linear terms, we showed the limitations of the linear approximation, which can lead to erroneous interpretation of experimental results in respect to the value of the in-plane correlation length and the wavelength dependence of roughness replication. Neutron GISAS experiments (Garching, FRM II) revealed non-isotropic roughness in neutron supermirrors and presence of two different length scale roughness components. Consequently, we have to modify the roughness models generally used for mirror analyses.

Investigation of willemite with different ions added. — The main parameters of willemite: Zn_2SiO_4, trigonal, R3, with hexagonal axes: a =13.948(2) Å, c = 9.315(2) Å, Z= 18, D_x = 4.224 $g \cdot cm^{-3}$. The structure of willemite has been refined by Rietveld method and an R value of 0.032 was achieved for powder samples.

The addition of different ions creates color centers in willemite, making it a good luminophore powder. The treatment of addition of ions can be processed by a high-temperature thermal dry way or a newly discovered low-temperature wet treatment. One of the goals was to check the result of the new treatment and to obtain accurate atomic parameters in order to provide a structural basis for the evaluation of the optical properties of willemite.

By the combined use of neutron and X-ray diffraction, we could determine that the different metallic ions are built in in a different way. Some of them created a separate phase (Ce, Eu), some of them could be built into the original willemite structure (Mn, Tb).

Characterisation of forming techniques and firing temperatures of archaeological ceramic artefacts. — Neutron tomography experiments on archaeological and experimental reference samples have been performed at the RAD instrument of the Budapest Neutron Centre. The aim of the project was to investigate the suitability of non-destructive neutron computer tomography as a means for identifying the forming techniques used in the production of ancient organic-tempered pottery. Specifically, it was aimed at creating a three-dimensional (3D) model of the distribution of the voids/carbonised particles left within the ceramic matrix resulting from the complete or partial combustion of organic fibres within samples of ancient pottery and modern replicas. Through statistical analysis of the orientation of these fibrous voids/particles in 3D space, the preferential alignments were detected, which in turn correlated with suspected or known forming techniques. This information can be used to further refine the detection of preferential particle alignments by more conventional and cheaper methods, in particular by petrographic analysis of ceramic thin sections.

A new, systematic and larger set of investigated samples (36 samples from 3 geological sources, 12 different firing temperatures between 500°C and 1000°C) and archaeological samples (12 samples from Keszthely, Hungary) have been measured at the Yellow Submarine and F-SANS instruments of the Budapest Neutron Centre in order to determine the correlation between the maximum firing temperature of the ceramic materials and the Porod exponent gained from the SANS measurements. Previous experiments on a smaller set of samples have already shown linear dependence between the maximum firing temperature and the SANS curves. Therefore, the main objectives of the new experiments were to examine 1) whether the aforementioned linear dependence only applies to a certain range of firing temperatures and 2) how clays from different geological sources correlate to each other. Our results show that the linear dependence can be observed between 550°C and 950°C, which might be explained by the mineral phase transitions and vitrification occurring in this range of temperatures. Clays from different geological origins, while displaying linear temperature dependency, show different levels of the power exponent – firing temperature master curves. These findings reveal the possibility to identify the characteristic processing temperatures at different provenances of the clay artifacts, after performing an extensive calibration of the SANS data using local reference samples.

Time-of-flight neutron diffraction (TOF-ND) analysis of Late Bronze Age metallic artifacts. — As a member of "Momentum Mobility research team" (From bones, bronzes and sites to society: Multidisciplinary analysis of human mobility and social changes in Bronze Age Hungary (2500–1500 BC), http://mobilitas.ri.btk.mta.hu), György Káli has investigated several sets of finds, especially bronze weapons and jewelry items from the Carpathian Basin. The tests covered the phase compositions, chemical distributions, preferred orientations and dislocation densities of the alloys to unfold the manufacturing techniques. These pieces of information are of great help for the archeology and historical sciences to determine the social, cultural and trade links between distant regions of a given period.

Other archaeometric investigations. — As participants of the IPERION CH (Integrated Platform for the European Research Infrastructure On Cultural Heritage) project, we have performed a large set of neutron diffraction studies in various fields (ancient metal, ceramic and other objects).

Study of oriental and European carbon steel swords (Iperion). — Earlier, we have shown that the oriented distribution of cementite inclusions is a very efficient resource for the sorting of steels produced by different forging techniques. Besides that, texture and stress analyses have been performed on the ferrite phase as well on a large set of samples from several European collections. These non-destructively gained results on the sample bulk are very helpful to the archaeo-metallurgists to unfold the medieval steel production techniques.

The 'Budapest Horse': A comprehensive technical investigation has been performed on the world-famous statuette called Budapest Horse and Rider attributed to Leonardo da Vinci. This small bronze of the Budapest Museum of Fine Arts was taken first in 2017 to the BNC to carry out non-destructive experiments to collect new information on the inside of both parts. Now PGAA and widespread neutron diffraction analyses have been performed. For that, two new detector banks have been installed to the TOF beam. A normal (90°) and a reversed one on the opposite side for diffraction tomography. Our results – of major international interest in the light of the investigations performed in the Washington National Gallery of Art in 2009 – will be published soon.

Grants

H2020-INFRADEV-1-2015-1: 676548 - BrightnESS - Building a research infrastructure and synergies for highest scientific impact on ESS (L. Rosta, 2015-2018)

H2020-IPERION CH-2014-2015: 654028 (L. Rosta, 2015-2019)

H2020-654000, SINE2020 Science & Innovation with Neutrons in Europe in 2020 Training (L. Rosta, 2015-2019)

International cooperation

HAS Romania Academic exchange, Institute of Chemistry Timisoara

HAS Romania Academic exchange, Institute of Physical Chemistry Bucharest

TéT Bilateral Project, Université Pierre et Marie Curie, Paris

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See also: R-J.6, R-K.2

S-M. Neutron optics

Alex Szakál, János Füzi, Zoltán László[#], Márton Markó, Ferenc Mezei[A]

Neutron instrumentation development. — Our group contributes to the Europen Spallation project by designing and delivering neutron optical components for the instruments. The NMX instrument is one ot those instruments where significant Hungarian contribution was delivered. The NMX instrument is a macromolecular single crystal time-of-flight diffractometer. The instrument has the length of 160 m to be able to use the full pulse of ESS (2.76 ms). The neutron guide system of the instrument has to transport the "useful" neutrons - reaching the maximum 0.5 cm large sample within 0.4^{o} total divergence - with high efficiency. In order to avoid the background caused by the fast neutrons and to decrease the cost of shielding, the beam has to go out of the line of sight within 24.5 m, i.e., before the inner surface of the bunker built to stop the energetic neutrons (up to 2 GeV). The original guide design of NMX consisted of a curved part until 24.5 m, and a straight one with the cross section of 3x3 cm^2. We developed a calculation method for the loss due to the imperfectness of the neutron guide system waviness and the misalignments of the mirrors. The results show that almost half of the beam will be lost in the original guide. The neutron loss can be avoided by applying the so-called ballistic guide, i.e., a guide system with diverging - straight - focusing sections. After the curved section, the divergence of the neutron beam is decreased with a diverging segment, then a long, ~100 m straight guide with larger (4.5x4.5 cm^2) cross section results more than two times less reflection in the guide, finally a parabolic focusing section focuses the beam onto the small sample. Since the curvature of the guide is horizontal, vertically the diverging section is already at the beginning of the guide system. To decrease the effect of the inhomogeneity and position-dependent divergence caused by the simple curved guide, the horizontal diverging part is asymmetric, the outer side (convex side in the curved region) of the guide after the curved section is diverging while the inner part goes parallel with the main beam in the first 3.5 m and then starts to diverge. With these modifications, the transmission of the guide could be increased to over 85%.

Beside the NMX instrument, we took part in the design of two other instruments at ESS: the BIFROST instrument is an indirect-geometry inelastic spectrometer optimized for extreme environments (high fields, low temperature, high pressure etc.) where the vertical divergence of the scattered neutrons is limited by the sample environment. We took part in the optimization of the chopper and analyser system of the instrument. The MIRACLES instrument is also an indirect-geometry inelastic spectrometer, a so called time-of-flight backscattering spectrometer for the investigation of slow changes like diffusion, low energy excitations etc. We took part in the design of the radial collimator system (around the sample) which reduces the background of the measurement.

[#] Ph.D student

Members of the group actively contributed to the fulfillment of the EU-H2020 BrightnESS project, including the development of a 2D position sensitive neutron detector with solid boron converter and the main components (bench, choppers, mask with pinhole) of the ESS Test Beam Line, dedicated to energy-sensitive imaging of the cold-neutron moderator. The chopper of the instrument is shown in Fig. 1. This equipment is expected to be the first instrument to receive neutrons and experimentally assess the performance of the low-dimensional moderator, initially proposed by Ferenc Mezei and implemented for the first time at ESS. A prototype of the equipment has been applied to map the energy-dependent brightness of the cold moderator at the Budapest Research Reactor as well as at the **J**EEP II reactor of IFE at Kjeller, Norway.

Figure 1. *The chopper and positioning sytem of the ESS Test Beam Line.*

Our group was part of the organizers and lecturers of the 12th Central European Training School on Neutron Techniques (CETS2018), which provided insight into neutron scattering and imaging techniques and their application for studies on structure and dynamics of condensed matter. An important mission of the school is to illustrate the multifarious neutron research potential towards higher education, academy and industry.

Grants

H2020-INFRADEV-1-2015-1: 676548 - BrightnESS - Building a research infrastructure and synergies for highest scientific impact on ESS (L. Rosta, 2015-2018)

International cooperation

European Spallation Source ERIC, Paul Scherrer Institute, Technical University of Denmark, École Polytechnique Fédérale de Lausanne, Niels Bohr Institute, Jeremiah Horwocks Institute, University of Messina, Helmholtz Zentrum Berlin, Forschungzenrum Jülich

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See also: R-J.6, S-L.2, S-L.5

✝ Deceased

S-N. Laser applications and optical measurement techniques

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Aerosol drug delivery/deposition in human lungs – *In vitro* experimental and *in silico* numerical simulation methods were used for the determination of the deposition distribution and deposition efficiency of aerosol drugs from pressurized metered dose inhalers and dry powder inhalers (widely utilized in the therapy of chronic pulmonary diseases) as a function of standard breathing parameters. The mass median aerodynamic diameter of the released particles was determined for different idealized inhalation waveforms, directly from the inhaler and after a realistic upper airway model. We found that the mass median aerodynamic diameter varies by a factor of 2 and decreases with increasing peak inspiratory flow and inhaled volume. It was measured to be approximately 10% lower after the upper airway. The stochastic lung deposition model was used to calculate the lung deposition of the medicament with each inhalation profile, taking into account the measured size distribution. We determined the minimum required inhalation flow for the examined dry powder inhalers for an acceptable level of lung deposition dose. Above 60 L/min peak inspiratory flow the lung deposition increases to above 50%, which may support a sufficient therapy. Our measurements showed that the length of the inhalation does not influence the lung deposition dose; peak inspiratory flow and inhaled volume are much more relevant factors. We presented a map of the deposition of the examined aerosol drug in the lung as a function of inhalation time and peak inspiratory flow (Fig.1.), which could be a useful tool for the doctors in the selection of the appropriate inhalation drug by knowing the correct inhalation parameters of the patient, these can help in the elaboration of personalized treatment.

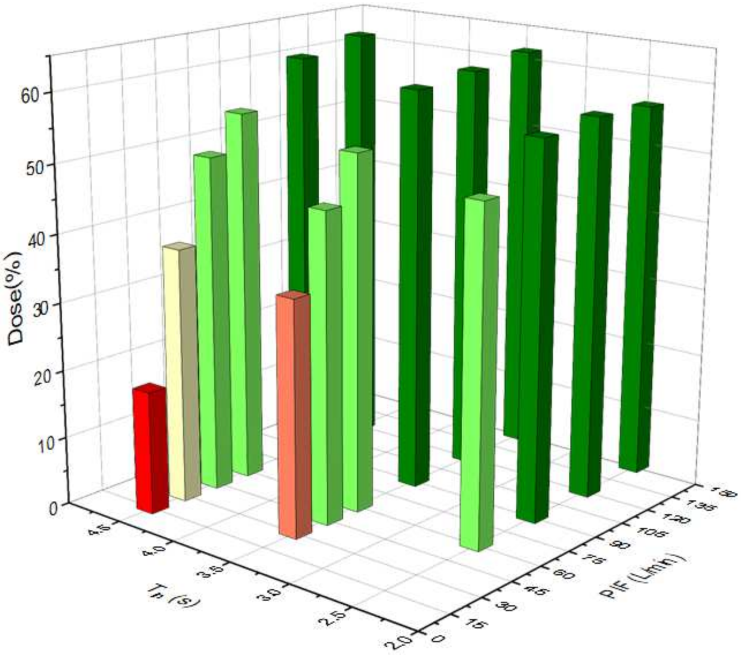

Figure 1. *The deposition efficiency map of a dry powder inhaler as a function of inhalation time (t_{in}) and peak inspiratory flow (PIF).*

Optical measurement techniques. — We have been involved in the development of prototype instruments for medical surgery applications based on short pulse and fibre lasers. The light scattering and absorption properties of model tissue materials were studied using

[A] Associate fellow

different lasers and detection techniques, as well as the aerosol plume that is generated upon the interaction of intense laser light and model tissue materials. The spreading, concentration and optical properties of the smoke was studied using high-speed cameras and non-contact laser Doppler methods. We have been participating in the development of a new technology based on 3D metal printing with industrial partners.

Our previously developed optical method was utilized in a research project aimed at investigating the properties of absorbing aerosols (mineral dust - black carbon mixtures) in the Mediterranean region. The main aims of the project are to characterize the aging and mixing of light-absorbing aerosol layers, to assess the contribution of individual aerosol components to the radiative forcing of mixed absorbing aerosol layers, to implement complex particle morphologies in radiative forcing estimates, and to investigate potential links between the presence of absorbing particles, aerosol layer lifetime and removal. Our instrument was installed into a research aircraft monitoring the vertical and horizontal profile of aerosol contamination of the atmosphere in given trajectories.

The development of light sources of our patented expanded-beam imaging Spectro-ellipsometers are in progress in co-operation with the Institute for Technical Physics and Materials Science, Centre for Energy Research. Bio-photonic research was conducted to optimize the label-free, in-vivo fluorescence emission of different biological samples, according to their individual destruction thresholds in order to develop an optimal excitation laser source.

Grants

EAC - European Aerosol Conference (A. Czitrovszky)

LASRAM Engineering - Wigner RCP Development of medical laser systems using fibre lasers and femtoseconds pulse lasers (A. Nagy, A. Czitrovszky 2016-2018)

2017-1.3.1-VKE-2017-00039: Unit production technology digitalization in the co-operation of Csepel Machine Tools Ltd., Lasram Engineering Ltd. and HAS Wigner Research Centre for Physics (A. Nagy, A. Czitrovszky 2018-2019)

International cooperation

University of Vienna (A. Nagy – W.W. Szymanski), Study of optical properties of aerosols and their climate relevance with dual wavelength optical particle spectrometer

University of Vienna (A. Nagy – B. Weinzierl), ERC Absorbing aerosol layers in a changing climate: aging, lifetime and dynamics (A-LIFE) project

Max Planck Institute of Quantum Optics (Garching, Germany) (A. Czitrovszky — F. Krausz), Study of ultrafast light-matter interactions.

Uzhhorod National University (Uzhhorod, Ukraine), (A. Czitrovszky)

Publications

Articles

1. Belyanin GA, Kramers JD, Andreoli MAG, Greco F, Gucsik A, Makhubela TV, Przybylowicz WJ, Wiedenbeck M: Petrography of the carbonaceous, diamond-bearing

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See also: R-L.2, S-R.3

S-O. Femtosecond lasers for non-linear microscopy

Róbert Szipőcs, Szabolcs Borzsányi, Luca Fésüs[#], Norbert Kiss[#]**,** Ádám Krolopp

CARS microscopy; Stain-free histopathology. — Basal cell carcinoma (BCC) is the most common malignancy in Caucasians. Nonlinear microscopy has been previously utilized for the imaging of BCC, but the captured images do not correlate with standard H&E staining. Last year, we have developed a novel algorithm to post-process images obtained from dual vibration resonance frequency (DVRF) CARS measurements to acquire high-quality pseudo H&E images of BCC samples. We adapted our CARS setup to utilize the distinct vibrational properties of CH_3 (mainly in proteins) and CH_2 bonds (primarily in lipids). As a result, we acquired two images: one for “lipids” and one for ”proteins” when we properly set a multiplication factor to minimize the non-specific background. By merging these images, we obtained high contrast H&E “stained” images of BBCs. Nonlinear microscope systems upgraded for real time DVRF CARS measurements providing pseudo H&E images can be suitable for *in vivo* assessment of BCC in the future.

This year, we introduced a fast and cost-efficient spectral modulation technique (IF-CARS) for sub-100 fs pulse Ti-sapphire lasers, which allows us to modulate the laser spectrum on a ms time scale with the use of a piezo-driven Michelson interferometer. Switching between the properly shaped “on-resonance” and “off-resonance” laser spectra can be synchronized either to the electronic “line” or to the “frame” signals of our laser scanning microscope, which allows us to perform real time non-resonant background suppression during CARS imaging. It might have applications in brain research, e.g., when investigating myelin breakdown in murine models with multiple sclerosis (MS). In an alternative setting, we modulate the laser spectrum in such a way that CARS imaging for “lipids” and “proteins” does not require the tuning of our pump laser or readjustment of the time delay, which paves the way for real-time stain-free histopathology.

We started from our CARS imaging setup referenced above, which received the Applied Research Prize of Wigner SZFI in 2015. For our IF-CARS experiments, we constructed a small size Michelson interferometer (see Fig. 1). In the beam path of the Ti:sapphire laser, we replaced one of the 45-degree folding mirrors by our small-size interferometer. One of its mirrors (M2) was placed on a piezo-electric linear actuator. The optical path difference ($2*\Delta L$) had an offset value of ~0.1 mm, which resulted in different modulated laser spectra at the interferometer output, depending on the phase difference of the two arms. For our stain-free histopathology imaging experiments on in vitro brain slices, we used different interferometer settings: we switched the phase difference between $\pi/2$ and - $\pi/2$ at the laser central wavelength of 975 nm. As a result, we obtained two wavelength-shifted laser spectra with maxima at 793 and 796 nm corresponding to the vibrational resonance of CH_3 (mainly in proteins) and CH_2 bonds (primarily in lipids).

[#] Ph.D student

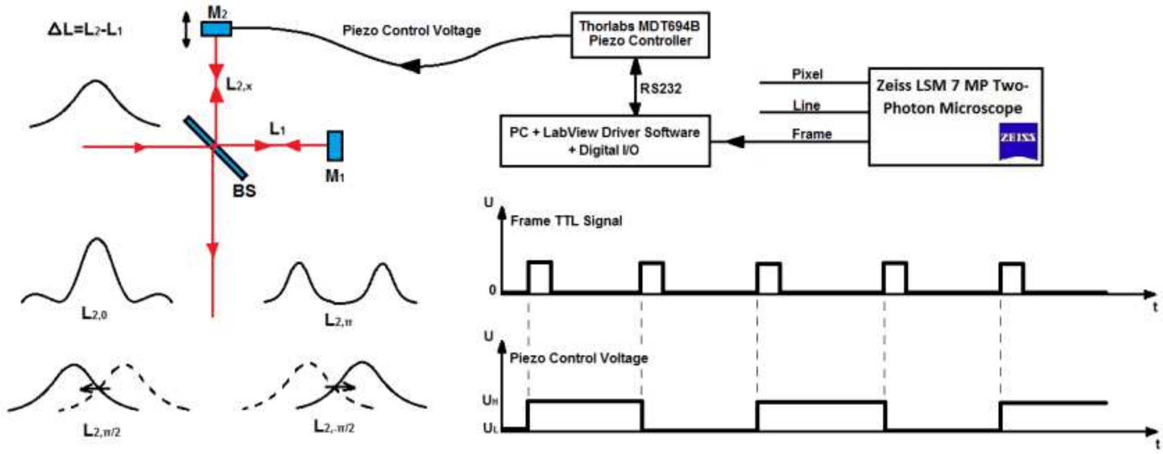

Figure 1. *A Michelson-interferometer is used for spectral modulation of the pump pulses. Depending on the electronically controlled phase difference of the two arms, different spectra can be generated for CARS imaging. ΔL has a properly set offset value depending on the spectral bandwidth of the laser applied. The phase difference is electronically controlled and synchronized to the frame signal of our microscope.*

In the following, we show representative images recorded from in vitro brain slices using this settings.

Myelin sheaths – wrapping around the axons of neurons – are rich in lipid; therefore we can record high-quality 3D CARS images. Degradation of the myelin sheath is the cause of neurodegenerative diseases such as multiple sclerosis (MS), but a clear mechanistic understanding of myelin loss is missing. Previously, we studied myelin breakdown in murine models with multiple sclerosis (MS) using the toxin cuprizone. We found that myelin debris form lipid droplets alongside myelinated axon fibers. For automatic lipid reconstruction, a strong and specific lipid signal is needed. Therefore, to exclude CH_3 signal originating primarily from proteins and non-resonant background, we introduced spectral modulation with our interferometer. Our results are summarized in Fig. 2.

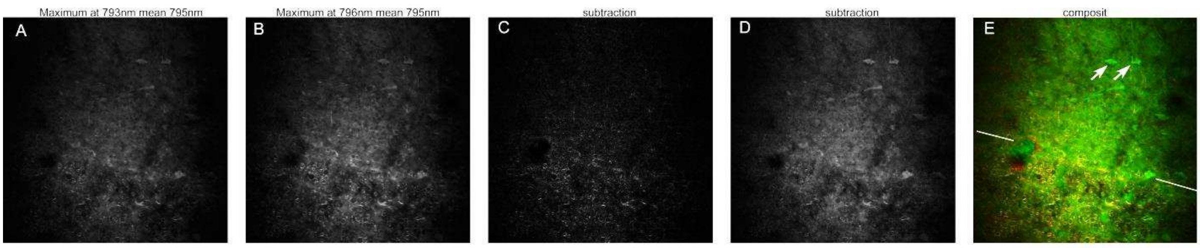

Figure 2. *IF-CARS imaging of in vitro brain slices with a Mai Tai pump laser tuned to 795 nm. A-B) Images of somatosensory cortex coronal slices of layer 6 and white matter were recorded for two different, spectrally modulated pump pulses with spectral maxima at 793 nm ("CH_3") and 796 nm ("CH_2"). C) Subtraction of images (CH_2 - CH_3) highlights more lipid structures. D) Inverse image subtraction (CH_3- CH_2) reveals protein rich background and somata of neurons. E) Composit image of lipid (red, CH_2- CH_3) and protein (green, CH_3-CH_2). Arrows show somata of neurons in layer 6, sidelong lines show the border of layer 6 and the white matter.*

Analysis of quantitative parameters in images of the collagen structure of basal cell carcinoma from SHG microscopy. — BCCs often have poorly defined borders, the clinical assessment of the tumor margins can be challenging. Therefore, there is an emerging demand for efficient *in vivo* imaging techniques for the evaluation of the tumor borders of BCC prior to and during surgeries. This demand might be met in the near future by nonlinear microscope techniques (such as second-harmonic generation (SHG) mosaic imaging) utilizing our novel, fiber-laser based, hand-held 3D nonlinear microscope system (*FiberScope*), which received the Applied Research Prize of Wigner SZFI in 2017. This year, we compared various quantitative parameters and algorithms for the analysis of SHG images of collagen in ex vivo human BCC and healthy skin samples to evaluate the utility of these methods in the detection of BCC.

Among others, we performed Fast Fourier Transformation (FFT) on the SHG images and converted the output of FFT into power plots. We fitted an ellipse to the power plots and collagen orientation index (COI) was calculated by COI = [1-(short axis/long axis)]. A COI value close to 0 reflects a normal sample with isotropic behavior, while a value close to 1 suggests parallel oriented fibers. Collagen bundle packing (CBP) was expressed as CPB = 512*(1/*h*), where *h* is the distance between the centers of gravity of two first-order maxima of FFT plots. FFT analysis was performed by ImageJ software (NIH, USA). FFT images of BCC displayed significantly higher COI, indicating that the collagen fibers are less randomly arranged, while no difference was found in the CBP value (Fig. 3). In the future, our novel image analysis methods (such as the FFT method briefly introduced here) could be integrated in our hand-held non-linear microscope system for sensitive and specific identification of BCC that, in longer term, can result in different applications such as surgery by robots.

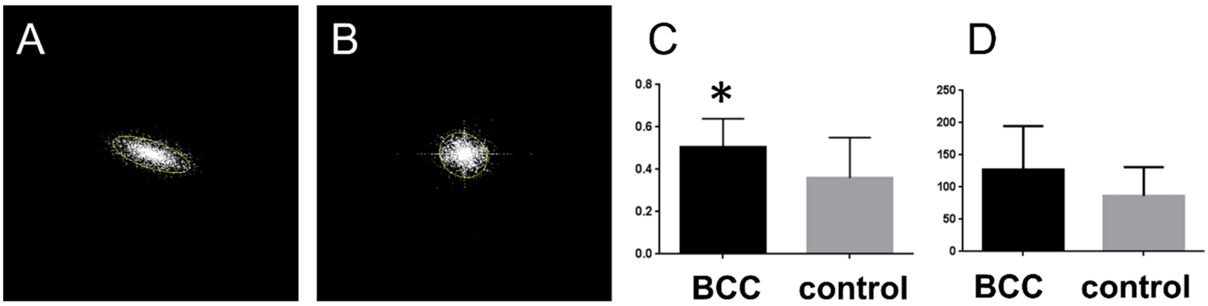

Figure 3. *A-B panels: Power plots of fast-Fourier-transformed second-harmonic generation images. A: basal cell carcinoma (BCC), B: control skin; C: collagen orientation index; D: collagen bundle packing. Error bars represent standard deviation, *p<0.05.*

Characterization of DHEA-induced PCOS-model by CARS microscopy. — Polycystic ovary syndrome (PCOS) is one of most frequent female endocrine disorder, affecting 5%–10% of women, causing infertility, disfunctional follicular maturation and ovulation, multicystic ovaries, hyperandrogenism. PCOS play a role in the enhancement of the risk of cardiovascular diseases and the development of diabetes. Postnatal treatment of rodents with DHEA (Dehydroepiandrosterone) induced human PCOS characteristics of acyclicity, anovulation, polycystic ovaries, and hyperandrogenism: DHEA induces ovarian cysts and causes abnormal hormon level (increased serum testosterone, androstenedione and 5-α-dihydrotestosterone) similar to the women with PCOS. Development of cysts causes an alteration of ovarian function and an imbalance in the oxidant–antioxidant balance. Increased reactive oxygen species (ROS) within ovarian cells is associated with the impaired ovarian function. DHEA transformed into potent estrogens such as estradiol and produces estrogenic effects of female sex hormone. Estradiol is involved in the regulation of the female reproductive cycles and responsible for the development of female secondary sexual characteristics such as the breasts, widening of the hips, and a feminine pattern of fat distribution in women. Mouse cumulus oocyte complexes (COCs) exhibit lipotoxicity responses in association with obesity or following treatment with high levels of *lipids in vitro*. Traditional medicine, marjoram herb (*Origanum majorana*) tea was found to improve insulin sensitivity and reduce the levels of adrenal androgens in the hormonal profile of PCOS women in a randomised, double-blind, placebo-controlled trial. Spearmint (*Mentha spicata)* has treatment potential on PCOS through inhibition of testosterone and restoration of follicular development in ovarian tissue. In our recent study, we have investigated the effects of pure 100 % natural essential oil mix of *Origanum majorana* and *Mentha piperita* in DHEA-induced PCOS-model by nonlinear microscopy, the results of which are summarized below.

4 week-old (~18 g) female C57 bl/6 mice were kept at 22 ± 2 °C under a 12 h light/12 h darkness cycle. The animals were fed normal diet and water was available *ad libidum*. C57BL/6 female mice were treated with dehydroepiandrosteron (DHEA) daily (6 mg/100 g body weight in 0.1 ml oil subcutan) for 20 consecutive days. The DHEA treated animals were randomized into different treatment groups (n=6): DHEA-K group and DHEA + Essential oil mix group. The latter group, after a DHEA treatment, was subsequently treated *per os* for 10 consecutive days with water solution of *Origanum majorana (150 mg/kg$^{body\ mass}$*, CAS 84082-58-6*)* and *Mentha piperita (20 mg/kg$^{body\ mass}$,* CAS 8006-90-4*)* essential oils. After 20 days DHEA and 10 days Essential oil mix treatment, the mice were injected intraperitoneally (i.p.) with PMSG (pregnant mare's serum) at 5 IU/12 g of body weight, followed 48 h later by i.p. injection of hCG (human chorionic gonadotropin) at 5 IU/12 g of body weight. The ovaries were dissected and COCs were isolated from the oviducts at 16 h after hCG injection, placed in HEPES-buffered α-MEM (5 % FBS) and counted under microscope. The COCs were stained by Bodipy for lipid content or by MitoSOX Red, which is a mitochondrial superoxide indicator. During the staining procedure manufacturer's instructions was followed. After washing steps, the COCs were fixed by paraformaldehyde. We used a 2PEF and CARS imaging setup similar to that described above.

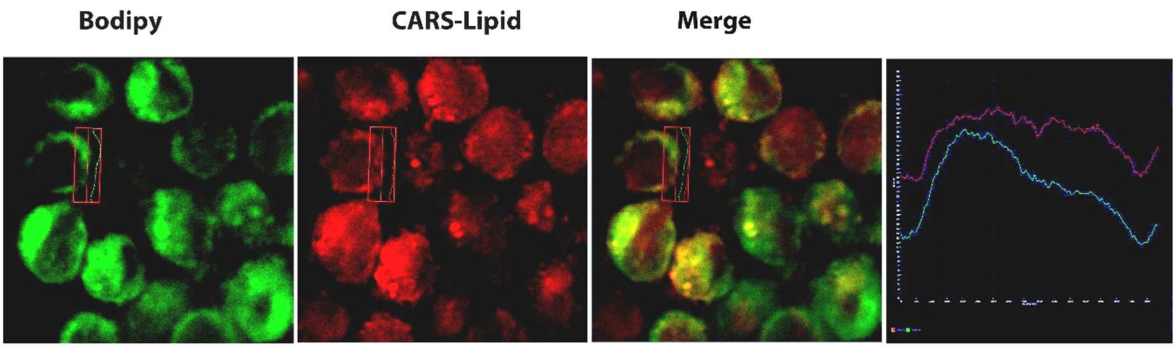

Figure 4. *Bodipy staining is concentrated mainly into the cytosol, which shows a clear co-localization with the detected CARS-lipid signal. Interestingly, the CARS image shows slightly higher spatial resolution than the corresponding 2PEF image.*

As a first step, we checked the co-localization of Bodipy fluorescent labelling and the detected CARS-lipid signal (see Fig.4). We found that even the small lipid droplets in the cells are clearly seen in both pictures. Interestingly, the CARS image shows slightly higher spatial resolution than the 2PEF image. As a next step, we compared the DHEA-induced changes of lipid content and ROS-level in COCs of murine PCOS-model by label-free CARS and MitoSox Red-labelled 2PE fluorescence microscopy (see Fig. 5). We found that DHEA treatment of female mice results in elevated lipid concentration of COCs parallel with increased mitochondrial ROS-production. Essential oil-mix treatment of mice decreased lipid and mitochondrial ROS-level in COCs. According to these results, we dare to say that CARS imaging might be a plausible approach to examine the effects of drugs on murine PCOS DHEA-model.

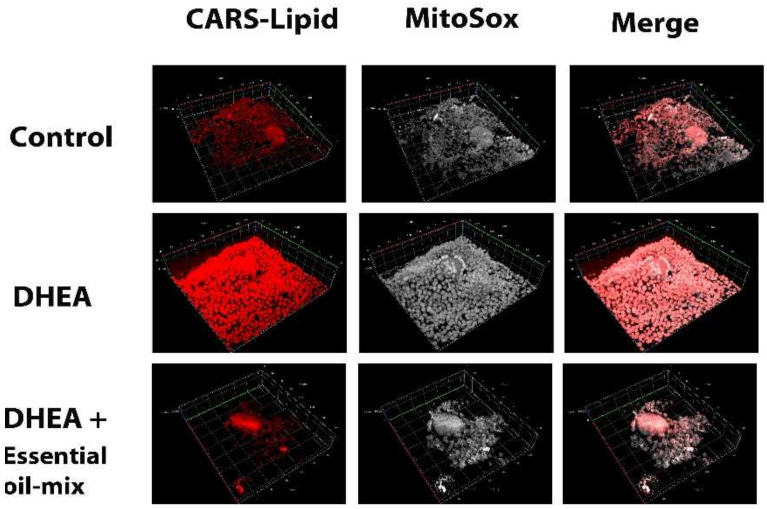

Figure 5. *Comparision of DHEA-induced changes of lipid content and ROS level in COCs of murine PCOS-model by label-free CARS and MitoSox Red-labelled 2PE fluorescence microscopy.*

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NKFIH K 129047 Advanced multi-wavelength ultrafast fiber lasers for stain-free histopathology (R. Szipőcs, 2018-2022)

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Biophotonics, Proc Biophotonics Congress: Biomedical Optics Congress 2018, (Microscopy/Translational/Brain/OTS), Hollywood, United States, 3–6 April 2018, OSA Publishing (2018) Paper: JW3A.12 2p

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S-Q. Crystal physics

László Kovács, László Bencs, Gábor Corradi[A], Gabriella Dravecz, Laura Kocsor[#], Krisztián Lengyel, Gábor Mandula, Ágnes Péter[A], Zsuzsanna Szaller, Éva Tichy-Rács[#]

$LiNbO_3$ single and nanocrystals. – A cost-effective, crucible-rest-refilling technology has been developed for the serial high-temperature top-seeded solid solution growth of high-quality Mg-doped stoichiometric $LiNbO_3$ crystals, resistant to optical damage. Nanocrystals have been prepared by shaker and planetary milling from $LiNbO_3$ crystals of congruent composition. While dry shaker milling resulted in particle sizes of a few hundred nm with gray coloration due to partial reduction, wet planetary milling with 0.1 mm zirconia balls in zirconia vial produced the desired 10-20 nm size.

Using EXAFS spectroscopy, the incorporation of Er, In and Hf dopants was determined in $LiNbO_3$ single crystals. Er mostly substitutes at the Li site with a small fraction at Nb site, with little change between stoichiometric and congruent $LiNbO_3$. In ions also primarily substitute at the Li site in congruent $LiNbO_3$; Hf appears to be nearly evenly distributed between Li and Nb sites. While charge-compensating defects are required, self-compensating schemes are not consistent with the data.

Using transient absorption spectroscopy in the mid/near infrared region in Mg-doped $LiNbO_3$ crystals, the dissociation and thermalization of hot excitons produced by 100 fs laser pulses at ~2.5 eV with power up to 2 PW/m^2 was shown to occur on a ~200 fs timescale leading to localized Nb^{4+} small polarons via an interim state attributed to electrons without local lattice relaxation. Exciton hopping and pinning on dipolar crystal defects have been demonstrated to play decisive roles in the luminescence components observed under pulsed excitation.

Spectroscopy of lithium yttrium orthoborate ($Li_6Y(BO_3)_3$, LYB) single crystals. – Undoped LYB single crystals grown by the Czochralski method were investigated for their suitability for optical applications. Two bands near the UV absorption edge, at about 220 and 240 nm, have been found with no and a small difference in their amplitudes between the top and bottom parts of the crystals for stoichiometric and off-stoichiometric compositions, respectively. XRF and luminescence measurements revealed no contamination of the crystals, so the UV bands can be attributed to intrinsic defects distributed more homogeneously in stoichiometric crystals.

The amplitude of the lowest energy absorption band of Yb^{3+} ions in LYB single crystals was observed to increase upon cooling from 300 to 9 K by more than two orders of magnitude, while the halfwidth decreased to 0.16 cm^{-1}. This strong temperature dependence explains the anomalous behavior of the time and intensity dependence of the cooperative pair emission previously investigated in similar crystals. Cooperative pair absorption was successfully demonstrated in a $Li_6Yb(BO_3)_3$ crystal (where Yb is a matrix ion) in the same wavenumber

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[A] Associate fellow

[#] Ph.D student

range where pair emission in LYB:Yb was observed. Spectral hole burning in LYB doped with monoisotopic $^{166}Er^{3+}$ ions has been investigated in magnetic fields. For coaxial field orientation, two pairs of spectral side holes were detected with a magnetic sensitivity of about ±75 and ±177 MHz/mT, while these holes split to more components in the case of a general direction of the magnetic field.

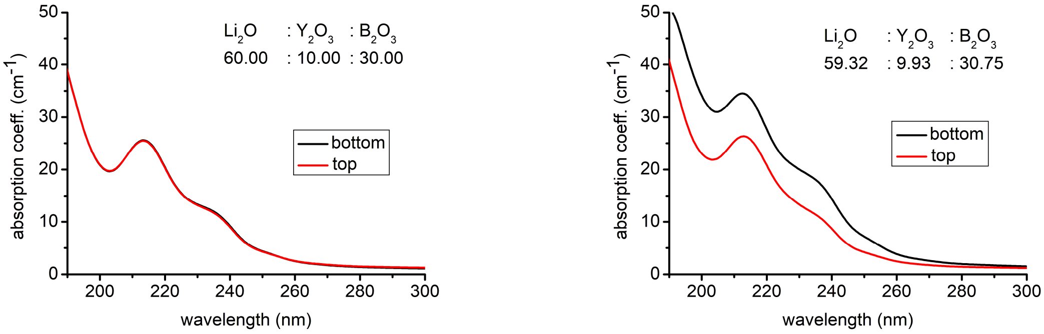

Figure 1. *UV spectra of slices cut from the top and bottom parts of stoichiometric and off-stoichiometric LYB crystals, the latter showing changed amplitudes.*

Designing and building a confocal microscope. – A new confocal microscope has been designed from the ground up to detect photons from a single-photon source. The samples mounted in a cryostat can be moved by synchronized motors. Optimal optical components were chosen for laser excitation and the detection of the emitted photons. A setup comprising a monochromator and a photon counter has also been developed for testing and optimizing solid state samples and suspensions.

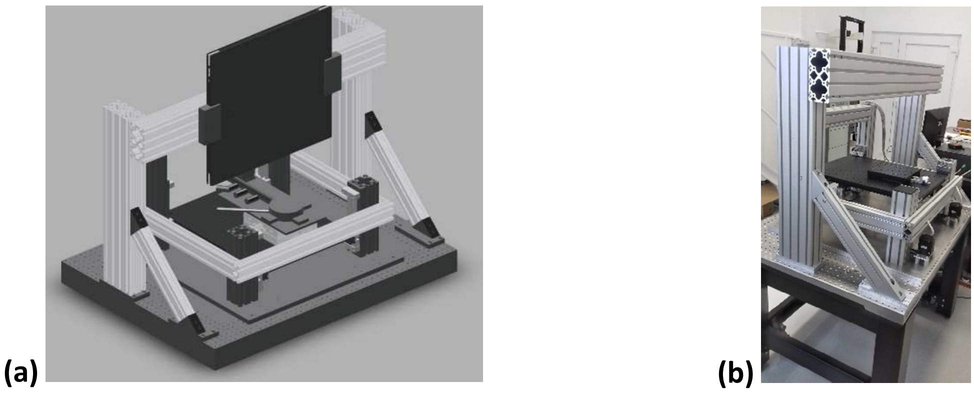

Figure 2. *Design (a) and realization (b) of the confocal microscope stand.*

Analytical methods for environmental and advanced materials. – An open-air ELCAD-OES system fitted with a low-resolution mini UV spectrometer has been built for on-line monitoring of river sediments. By correcting for structured molecular background emissions, the signal-to-noise ratios for Cd, Cu, Mg, Mn, Ni, Zn, etc. can be significantly improved. Acidic pressure digestion and flame atomic absorption methods were developed for major and minor constituents (Al, Ca, Fe, K, Mg, Mn, Na, Si, Sr, Ti) of alginite, which is an environmentally and agriculturally strategic mineral in Hungary.

Grants

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GINOP-2.2.1-15-2017-00037 (2018-2019, Application of national volcanic raw materials in environmental protection, consortium leader: BIOCENTRUM ltd., Gyöngyösoroszi, contributor: L. Bencs).

International cooperation

Tartu University (Estonia), Spectroscopy of doped borate crystals for quantum optics and dosimetry (G. Corradi, participants: L. Kovács, K. Lengyel and É. Tichy-Rács)

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S-R. Nanostructures and applied spectroscopy

Miklós Veres, Malik Al-Lami[#], Péter Baranyai, László Himics, Roman Holomb, Margit Koós[A], István Rigó[#], Sára Tóth, Tamás Váczi

Gold-catalyzed synthesis and structural characterization of a new type of As-S nanocrystallites. — Non-crystalline chalcogenides with high infrared transparency have stood out as materials of choice for infrared optics. Detailed studies of the physical properties of these materials revealed their unique and remarkable structural, electronic, optical properties and large functionality, and has attracted significant attention, representing an important scientific and technological challenge as well. They offer wide possibilities in domains such as information technologies (optical data storage, ultrafast optical transmission and information processing), photolithography, renewable energy technologies (high efficiency solar cells, solid electrolytes), medicine, thermal imaging, sensing and biosensing *etc.* Recent progress in photonics shows that amorphous chalcogenides are among the best candidates as active optical media for ultrafast *all-optical* processing systems.

Crucial differences were observed between the structure and properties of As-S chalcogenide thin films prepared by normal and gold-catalyzed thermally initiated vapor deposition from the same As_2S_3 glass precursor. The as-deposited As_2S_3 film prepared by thermal evaporation contains large concentrations of photosensitive realgar-like As_4S_4 inclusions compared to the structure of bulk As_2S_3 glass. The irradiation of this film by near- or over-bandgap coherent light initiates significant structural transformations connected mainly with induced transformation of realgar As_4S_4 molecules into their pararealgar polymorph. In contrast, formation of novel molecular nanocrystals was observed on the surface of As_2S_3 films synthesized with gold-catalysis. The size and shape of the crystallites was characterized by electron microscopy and their structure was found to be not photosensitive. Surface-enhanced Raman spectra of crystallites were interpreted with DFT calculations and showed that the crystallites are built from As_4S_5 cage-like molecules forming tetra-arsenic pentasulfide (Fig. 1).

Color centers in nanodiamond. — A gold-coated array of flow-through inverse pyramids applicable as substrate for entrapment and immobilization of microobjects and for their subsequent surface enhanced Raman spectroscopic (SERS) characterization was fabricated using bulk micromachining techniques from silicon. The inverse pyramids have 2.2x2.2 microns sized base on the top (being flush with the silicon surface) and a 0.5x0.5 micron-size opening on the bottom (Fig. 2). The perforated periodic 3D structure was demonstrated for parallel particle trapping and sensitive detection of molecules by entrapment and SERS characterization of polymeric microspheres. It was found that the periodic array has efficient near-field enhancement in the 650-850 nm region. Raman intensity maps recorded over the entrapped microspheres indicated efficient SERS enhancement inside the inverse pyramids.

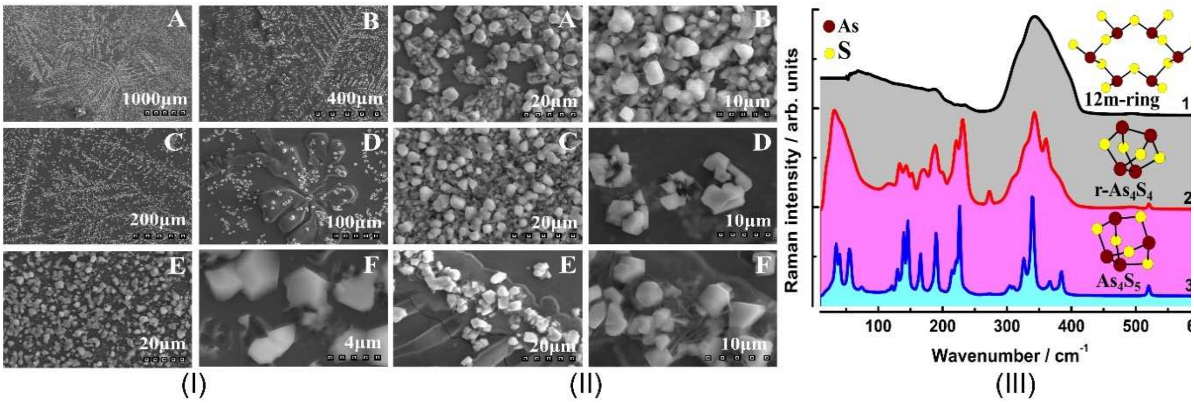

Figure 1. *(I) Surface morphology and distribution of As_4S_5 microcrystallites on As_2S_3 films synthesized by gold-catalyzed vapor deposition on 5-60 nm Au nanoparticles (A-F); (II) SEM images of As_2S_3 nanolayers synthesized with spherical gold nanoparticles of different size: 5 nm Au-np (A,B), 40 nm Au-np (C,D), and 60 nm Au-np (E,F); (III) FT-Raman spectrum of glassy As_2S_3 (1) and surface-enhanced Raman spectra of As-S thin films prepared by thermal deposition (2) and gold-catalyzed vapor deposition (3). The main cluster constituents of the films are also indicated on the Figure.*

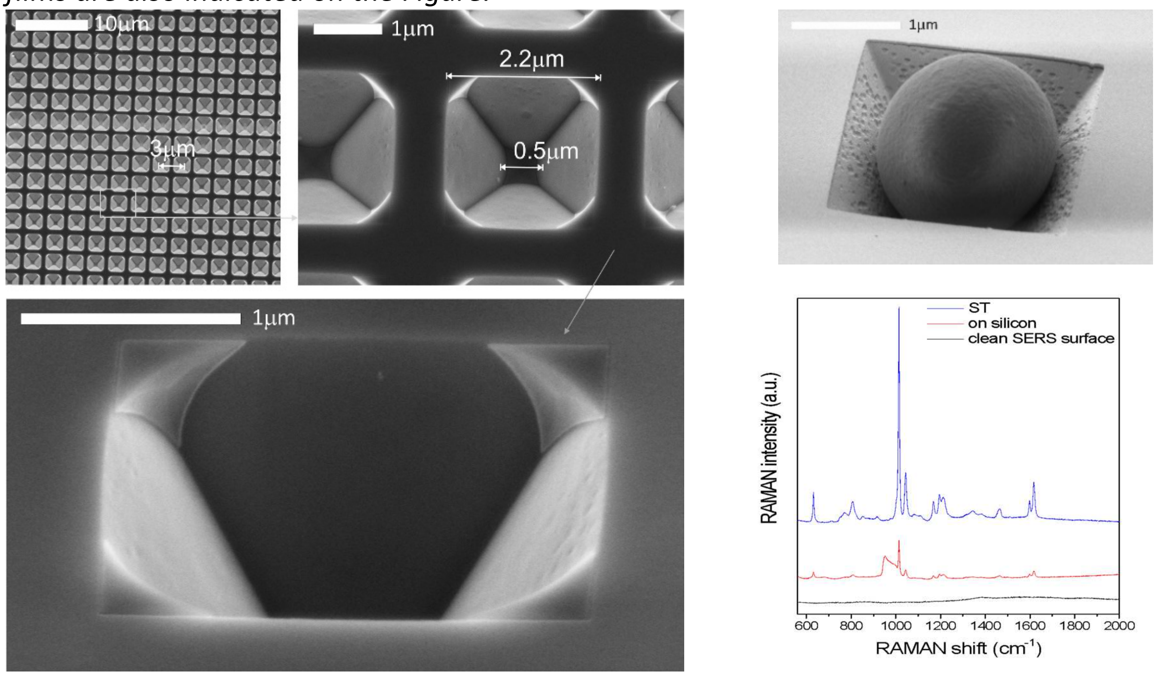

Figure 2. *SEM view of the periodic perforated SERS substrate applicable for flow-through experiments and particle and cell entrapment (left). Polymeric microparticle entrapped in an inverse pyramid of the SERS substrate (top right). Comparison of the SERS spectra recorded on the clean SERS surface and entrapped microparticle (ST) and normal Raman spectrum of the latter on silicon (bottom right).*

Grants

Bolyai János Scholarship of the HAS: Creation of light emitting color centers using novel techniques in diamond nanocrystals (S. Tóth, 2016-2019)

EU H2020 FET-Open: Visual genetics: establishment of a new discipline to visualize neuronal nuclear functions in real-time in intact nervous system by 4D Raman spectroscopy (M. Veres, 2016-2019)

H2020-MSCA-RISE-2016 VISGEN: Transcribing the processes of life: Visual Genetics (M. Veres, 2017-2021)

NVKP_16-1-2016-0043: Development of fluorescent dyes and high resolution, fast scanning 3D microscope for the treatment of epilepsy (M. Veres, 2017-2019)

VEKOP-2.3.2-16-2016-00011: Strategic workshop for the technological challenges of renewable energy systems (M. Veres, 2017-2020)

COST MP1401: Advanced fibre laser and coherent source as tools for society, manufacturing and life science (M. Veres, 2016-2018)

COST CA16101: MULTI-modal Imaging of FOREnsic SciEnce Evidence - tools for Forensic Science (M. Veres, 2017-2020)

International cooperation

University College London, Department of Chemistry, Christopher Ingold Laboratories, London UK (S. Tóth)

Saint Petersburg National Research University of Information Technologies, St. Petersburg, Russia (S. Tóth)

Universität Kassel, Kassel, Germany (L. Himics)

Uzhhorod National University, Uzhhorod, Ukraine (M. Veres)

V.E. Lashkaryov Institute of Semiconductor Physics, Kiev, Ukraine (M. Veres)

A.M. Prokhorov General Physics Institute, RAS, Moscow, Russia (M Veres)

University of Birmingham, Birmingham, United Kingdom (M. Veres)

Max Planck Institute for Neurobiology, Martinsried, Germany (M. Veres)

Institut für Mineralogie und Kristallographie, Universität Wien, Vienna, Austria (T. Váczi)

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See also: R-K.5

THE RESEARCH LIBRARY

Anikó Kutnyánszky, Szabolcs Bálint, Andrea Harsányi, Emese Szabó, Ilona Verle

The library's main task is to provide information resources and materials for the research centres and institutes of the Hungarian Academy of Sciences (HAS). Although it is jointly financed by the two user institutes (Centre for Energy Research and Wigner Research Centre for Physics), it is developed and managed by the Wigner Research Centre.

On 31 December 2018 the stock of the library consisted of 60 842 print monographs and conference proceedings, 1563 electronic books with remote access, 41 231 periodical issues and 40 893 research reports. From the 143 newly acquired print books that were added to the collection, 67 were purchased, 64 were donated, and 12 items were meant for provisional deposit. In addition, a total of 831 items were sorted out and removed from the collection.

From the library stock, 236 print items (books, journal issues and reports) were borrowed by more than 100 registered users on the campus, and the due date of 425 items was renewed during the year. In addition, 184 user requests were fulfilled by the library staff by downloading the online versions of articles or scanning printed materials.

Within inter-library loan services, 118 library items were provided to our registered users in either print or electronic format, and we successfully completed 51 document requests made by other libraries and external partners. In 2017, we had a network of 36 partner institutes in Hungary and abroad.

The Library had a subscription for 18 print periodical titles and the issues of 5 additional titles were donated to the library. There were 95 electronic journals with full-text access available for the researchers via individual subscriptions, and the library also had access to more than 14 000 online periodicals in the scientific databases sponsored by the Electronic Information Service National Programme (EISZ). As a new resource, the Library had subscribed for the EBSCO Applied Science and Technology collection in 2018.

Péter Lévai, director general of WRCP has become a member of the Programme Board of Electronic Information Service National Programme to represent the institutes of natural sciences in the network of research institutes of HAS.

To support authors in making their articles open access published in Royal Society of Chemistry journals, 3 vouchers have been used by authors from the Wigner Research Centre and 1 voucher from the Energy Research Centre. This program continues in the next year in partnership with more publishers.

As part of the retrospective conversion project, the library staff added as many as 8145 records of books to the library catalogue and with this, 58% of the Library stock are now completed in catalogue.

It was the first time to purchase e-book packages on the library's budget supported by EISZ. In 2018, collections were purchased from IOP (packages "Release 1-4 with AAS" which includes also a package of the American Astronomical Society, AAS) and from SpringerNature (packages "Physics & Astronomy 2017" and "Chemistry & Materials Science 2017"). A total of 1563 titles are available via institutional access at no additional charge. Other e-book collections were purchased via EISZ from Interkönyv Typotex with 552 Hungarian ebooks titles, where numerous books were written by our local academic authors from the campus. All contents are available for on-line use, although with limited downloading options.

With the help of an IT specialist, the website of the library has been updated and made accessible to the visually impaired.

On 9th May, 2018, an information day was organized by the library staff for those researchers on the Csillebérc campus who were interested in the overall services and the subscriptions of the library. Presentations were made in front of a group of about 15 people.

A successful event of GDPR workshop for corporate librarians was held on 7th June, in the Wigner Data Center hosted by the Wigner Library in partnership with the Association of Hungarian Librarians (MKE) where 31 participants attended.

Old letters and documents issued between 1952 and 1999 at the former Central Research Institute for Physics (KFKI), the predecessor of the Wigner Research Centre and the Energy Research Centre, were listed and handed over to the Archives of the Hungarian Academy of Sciences for archiving. The material arranged into 200 folders and labelled properly to make it available for research was taken to a storage in Törökbálint.

Digitization of archival footage and video recordings about KFKI that are part of the stock of the library have been completed. The films are being in the progress of editing and will prospectively be available to see on the institute's social media platforms and public internet platform.

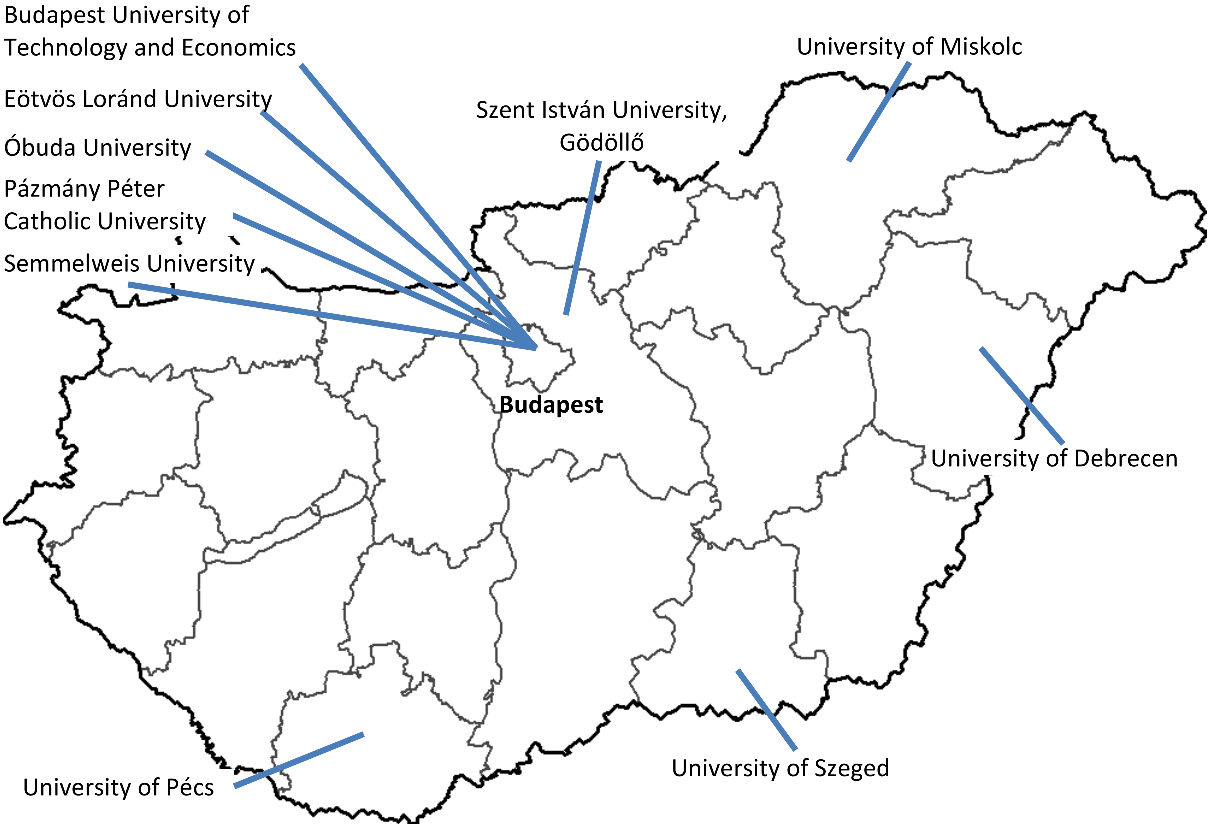
Former KFKI publications, 'KFKI Tájékoztató', 'KFKI Közlemények' and 'KFKI Yearbook' have been digitized in the first part of the digitization project of the Hungarian academic periodicals and materials and uploaded into the REAL Repository of the Library of HAS. Digitizing continues with processing the copies of 'KFKI Reports'. These online materials with full-text access will be available on Arcanum Digital Platform (ADTPLUS) presumably in 2019.

The Library staff participated in several professional events and conferences. The head of the library gave a presentation on the services of the Wigner Library on the annual meeting of the research libraries of HAS on 22nd February. She also attended the annual conference of the Association of Hungarian Librarians (MKE) in Keszthely. As part of a training programme, she completed an 8-day course on 'Performance evaluation and digital skills of librarians' organized by the National Széchényi Library (OSZK).

Members of the Library visited other libraries to exchange best practices: the Budapest Collection of Metropolitan Szabó Ervin Library; the Library of the **Geographical Institute at the Research Centre for Astronomy and Earth Science HAS; and the** HAS Centre for Social Sciences.

SUPPLEMENTARY DATA

Education



Graduate and post-graduate courses

Eötvös Loránd University, Budapest

- Advanced biostatistics (Z. Somogyvári)
- Algebraic quantum field theory (P. Vecsernyés)
- Cognitive neuroinformatics II, Budapest Semester in Cognitive Sciences (Z. Somogyári)
- Cognitive neuroscience, Budapest Semester in Cognitive Sciences, (L.Négyessy)
- Computational neuroscience (Z. Somogyvári)
- Electrodeposition of metals (L. Péter)
- Experimental methods of structure determinationI-II. (L. Temleitner)
- Integrable methods in the gauge/gravity duality I (Z. Bajnok)
- Introduction to cognitive science, Budapest Semester in Cognitive Sciences, (P. Érdi)
- Introduction to gravitational theory and high-energy physics (G.G. Barnaföldi, M. Vasúth)
- Introduction to general relativity (M. Vasúth)
- Investigation of the inner structure of compact stars (G.G. Barnaföldi)
- Macromolecules (S. Pekker)
- Many-body problem I-II. (G. Szirmai)
- Nanophase metals (I. Bakonyi)
- Neurophysiological data analysis (Z. Somogyvári)
- Neutron physics (M. Márton)
- Nuclear solid-sate physics I-II (D.L. Nagy)
- Optics and relativity theory (J. Cserti, Gy. Dávid, D. Varga)

- Physics of jets (P. Lévai)
- Physics of liquid crystals and polymers (Á. Buka and N. Éber)
- Physics of the solar system (Z. Németh)
- Plasma physics (Z. Donkó)
- Raman spectroscopy in Earth sciences (T. Váczi)
- Scientific programming for graphics processors I. (M.F. Nagy-Egri)
- Scientific programming for graphics processors II. (D. Berényi)
- Selected chapters from high-energy experimental physics (multiple lecturers, including A. László, D. Varga)
- Selected chapters on compact star interior (G.G. Barnaföldi)
- Selected topics in experimental high-energy physics (F. Siklér, R. Vértesi)
- Solid State Physics (I. Tüttő)
- Statistical physics (G. Szirmai)
- String Theory (Z. Bajnok)
- Superconductivity (I. Tüttő)
- The phase-structure of the strongly interacting matter (P. Lévai)
- Trends in materials science (Á. Gali)

Budapest University of Technology and Economics

- Coherent control of quantum systems (Z. Kis)
- Engineering thermodynamics II. (R. Kovács)
- Fusion devices (G. Veres)
- Fusion devices (G. Pokol)
- Group theory in solid state research (G. Kriza)
- Industrial systems diagnostics (G. Pokol, guest lecturer)
- Inertial confinement fusion (single lecture within the course "Introduction to the fusion plasma physics" of G. Pokol) (I. Földes)
- Infrared and Raman spectroscopy (K. Kamarás)
- Interacting spins in materials (K. Penc)
- Introduction to fusion plasma physics (G. Pokol, S. Zoletnik, D. Dunai)
- Introduction to irreversible thermodynamics (P. Ván)
- Introduction to superconductivity (G. Kriza)
- Introduction to theoretical plasma physics (A. Bencze)
- Investigation techniques for materials science (T. Keszthelyi)
- Mechanics I-II. (A. Virosztek)
- MHD in low dimensional systems (A. Bencze)
- Modern nuclear energy (G. Pokol)
- Modern solid state physics (A. Virosztek)
- Neutron physics (M. Márton)
- Nuclear fuel cycle (M. Fábián)
- Nuclear physics (G. Pokol, guest lecturer)
- Numerical simulations of caloric machines (R. Kovács)
- Plasma physics (Z. Donkó)
- Quantum entanglement (Sz. Szalay)
- Quantum optics (P. Domokos)

- Quantum optics (J.K. Asbóth)
- Spectroscopy and the structure of matter (K. Kamarás)
- Theoretical solid state physics (A. Virosztek)
- Theory of magnetism (A. Virosztek)
- Variational methods in the basics laws of physics (T.S. Biró)

Oulu University, Oulu, Finland

- Lecture course on nanophase metals with special view on spintronics (I. Bakonyi)

Óbuda University, Budapest

- Chemistry and physics of polymers (S. Pekker)

Pázmány Péter Catholic University

- Basic calculus (B. File)
- Neuoromorph movement control. (J. Laczkó)
- Research methods in sociology, (B. File)
- Webmining (B. File)

Subotica Tech - College of Applied Sciences (Serbia)

- Physics of enginiering, (F. Bazsó)

Semmelweis University, Budapest

- Learning and navigation, Systems Neuroscience Summer School, (Z. Somogyvári)
- Neocortex: from structure to function, Systems Neuroscience Summer School (L.Négyessy)
- Neuroinformatics (L. Négyessy, F. Bazsó, L. Zalányi, Z. Somogyvári)

Szent István University, Gödöllő

- Biophysics (I.F. Barna, in German)

University of Debrecen

- Particle physics 1 and 2 (D. Horváth)
- Particle physics exercises (D. Horváth)
- Structure and experimental test of the standard model 1 and 2 (D. Horváth)

University of Pécs

- Algebra and number theory II-III. (J. Laczkó)
- Control and regulation technology (J. Laczkó)
- Control systems (J. Füzi)
- Digital control (J. Füzi)
- Electronics (J. Füzi)
- Geometry and visualisation (J. Laczkó)
- Mechanics - dynamics (A Len)
- Neurobioinformatic programming (J. Laczkó)

- Numerical methods (P. Ádám)
- Open quantum systems (P. Ádám)
- Probability theory (P. Ádám)
- Quantum information processing by quantum optical means II. (T. Kiss)
- Resonant light-matter interaction (P. Ádám)
- Seismic design (A. Len)
- Statistical physics (K. Szlachányi)
- Theoretical mechanics (K. Szlachányi)
- Theoretical physics III (P. Ádám)

University of Szeged

- Analytical mechanics (L. Fehér)
- Applications of statistical physics (F. Iglói)
- Introduction to statistical physics (F. Iglói)
- Introduction to the physics of laser plasmas (I. Földes)
- Introduction to the theory of nonlinear laser-matter interactions (S. Varró)
- Modeling heavy-ion collisions (Gy. Wolf)
- Nuclear and particle physics (L. Fehér)
- Statistical physics (F. Iglói)
- Symmetries in physics (L. Fehér)
- The properties of dense, strongly interacting matter (Gy. Wolf)

University of Veterinary Medicine, Budapest

- Biophyics (Z. Szőkefalvi-Nagy, both in Hungarian and in English, two courses)

University of Warsaw, Poland

- On the use of evolutionary methods in metric theories of gravity (I. Rácz)

Laboratory practices and seminars

Eötvös Loránd University, Budapest

- Advanced physics laboratory (R. Vértesi)
- Atomic and molecular physics (P. Udvarhelyi)
- Differential equations in Physics II (T. Gombor)
- Electrodynamics (M. Lajer)
- Environmental radiations laboratory (G. Galgóczi)
- Experiments on liquid crystals (Á. Buka, N. Éber, P. Salamon, T. Tóth-Katona)
- IT tools for research (G. Biró, M.F. Nagy-Egri)
- Laboratory practice on neutron scattering (L. Almásy, A. Len, M. Fábián, L. Rosta, T. Veres, Gy. Török)
- Modern physics laboratory (P. Udvarhelyi)
- Nuclear techniques and X-ray spectroscopy (Z. Németh)
- Nuclear techniques for elemental analysis (RBS and ERDA), extended practice for physics students (E. Szilágyi)

- Particle, nuclear and astrophysics lab / MHD waves (A. Opitz)
- Particle and nuclear physics detectors laboratory (G. Hamar, D. Varga)
- Probability theory (M. Kornyik)
- Probability theory and statistics (M. Kornyik)
- Quantum mechanics (M. Lajer)
- Raman spectroscopy, part of the course Laboratory practice in biophysics (M. Veres)
- Statistical physics (G. Szirmai)

Budapest University of Technology and Economics

- Applied thermodynamics (R. Kovács)
- Engineering thermodynamics II (R. Kovács)
- Heat and flow transfer in mechatronics elements (R. Kovács)
- Independent task I-II. (L. Bencs)
- Individual project (D. Beke)
- Infrared and Raman spectroscopy (K. Kamarás)
- Introductory physics for chemical engineers (A. Csóré)
- Laboratory practice (M.A. Kedves, B. Ráczkevi)
- Laboratory practice on neutron scattering (L. Almásy, A. Len, M. Fábián, L. Rosta, T. Veres, Gy. Török)
- Nuclear- and neutron physics practical lesson (G. Nyitrai)
- Physics II for electrical engineers (A. Csóré)
- Physics II for informaticians (A. Csóré)
- Physics II. for IT students (A. Buzás)
- Quantum mechanics (Z. Kökényesi)
- Raman spectroscopy, part of the course Experimental methods in materials science (M. Veres)
- Remote measurement on the GOLEM tokamak (G. Pokol)
- SUMTRAIC Summer School (A. Bencze)
- Thermal physics, mechatronics I-II.(P. Ván)
- Thermodynamics and heat transfer (R. Kovács)

Eszterházy Károly University, Eger

- Statistics I. (G. Kasza)
- Statistics II. (G. Kasza)
- Mathematics for economy I. (G. Kasza)

Pázmány Péter Catholic University, Budapest

- Neuoromorph movement control (L. Botzheim)

Technical University, Dresden, Germany

- Quantum mechanics (G. Roósz)
- Statistical physics (G. Roósz)

University of Pécs

- Biorobotics (J. Laczkó)

- Control systems I-II (J. Füzi)
- Diagnostics – SEM laboratory practice (A. Len)
- Geometry and visualisation (J. Laczkó)
- Mathematical methods in physics IV. (D. Jakab)
- Mathematical methods in physics IV. (P. Ádám)
- Mechanics – dynamics - seminar (A. Len)
- Professional commuication (J. Laczkó)
- Probability theory (P. Ádám)

University of Szeged

- Summer practice in the HILL laboratory, high intensity laser-plasma interactions (I. Földes)
- Physics practice for 1st year BSc students and for 1st year MSc students (I. Földes, Zs. Kovács)
- Electronics laboratory (Zs. Kovács)
- Physics and biophysics laboratory practice (Zs.Kovács)

Diploma works

Eötvös Loránd University, Budapest

- B. Csurgai-Horváth, Modeling high-energy nuclear effects in HIJING++ (BSc, Supervisor: G.G. Barnaföldi, G. Papp, G. Bíró)
- A. Leitereg, Generative programming of massively parallel architectures (MSc, Supervisor: D. Berényi)
- D. Nagy, Development and testing of Monte Carlo code simulating heavy ion collisions (Bsc, Supervisors: G.G. Barnaföldi, G. Papp, G. Bíró)
- Á. Takács, Parton fragmentation in the non-extensive statistical model (Msc, Supervisors: G.G. Barnaföldi and G. Papp)
- A. Olár, Coalescence model development for transport models (Bsc, Supervisor: Gy. Wolf)
- Z. Pollyák, Rock mechanical analysis (BSc, Supervisor: P. Ván)
- O.B. Visnyei, DCS system for CERN LHC ALICE interface (MSc, Supervisors: Á Fülöp, G.G. Barnaföldi)
- A. Bodor, Finite size effects of form factors in integrable theories (MSc, supervisor: Z. Bajnok)
- I. Vona, Finite size effects of form factors in quantum field theories (MSc, supervisor: Z. Bajnok)
- B.E Szigeti, Studying the quark-gluon plasma with angular correlations (BSc, supervisor: M. Varga-Kőfaragó)
- P. Géczi, Muon tomography – or mapping of high-density materials by cosmic particles (BSc, supervisor: L. Oláh)
- A. Németh, Experimental determination of avalanche-starting efficiencies of GEM foils (MSc, supervisor: A. László)
- M. Novák, Numerical and experimental study of superconducting magnetic shields for the construction of a high field septum magnet (MSc, supervisor: D. Barna)
- K. Brunner, Improving the slow extraction efficiency of the CERN Super Proton Synchrotron (MSc, supervisor: D. Barna)

- P. Szebeni, The analysis of the economic and environmental aspects of fusion energy production in Hungary: (Supervisor: D. Dunai)
- Á. Madár, Predicting the solar wind and the interplanetary magnetic field for ESA Solar Orbiter (MSc, supervisor: A. Opitz)
- D. Herrmann, Temperature interpretation at different altitudes of the terrestrial atmosphere (MSc, supervisor: A. Opitz)
- Sz. Hegyesi, Characterizing the dispersion properties of inhalers by optical measurement techniques, (BSc, supervisor: Sz. Kugler)
- B. Lovász, Investigation of ultrafast photoelectrons emitted from nanoparticles (Supervisor P. Dombi, ELTE)
- D. Bugár, Quantum walk on lattices with nontrivial topology (BSc, supervisor: T. Kiss)

Budapest University of Technology and Economics

- G. Balassa, Multiple scattering in high-energy heavy-ion collisions (Msc, Supervisor: Gy. Wolf)
- D. Hermann, Finite element thermodynamical models of layered structure materials (Supervisor: R. Kovács)
- M. Mázsi, Gasturbine burner heat-distribution and cooling technologies, (BSc, Supervisor: P. Ván)
- G. Nyitrai, Mechanical analysis of a detector scanner (MSc, supervisor: D. Varga)
- A. Vancza, Relaxation dynamics of an optically excited Fe(II) complex studied by ultrafast spectroscopy, (B.Sc., supervisor: T. Keszthelyi)
- Á.D. Major, Marking proteins with silicon-carbide nanocrystals (MSc, supervisor: D. Beke)
- S. Szabó, Quantum mechanical simulations of the silicon vacancy in silicon carbide (BSc, supervisor: Á. Gali, BME)
- V. Nagy, Detection of flow fields by digital image analysis (BSc, supervisor: T. Börzsönyi)
- Trần Quang Thiện, Effect of bi- and trivalent doping ions, on the sol-gel derived zinc silicate structural properties (MSc, supervisors: Gy. Török and Z. Dudás)
- P. Kárpáti, Optimization of neutron guide systems (MsC, supervisor: M. Markó)
- B. Éles, Ultrafast photoemission from plasmonic metal structures (Supervisor P. Rácz, BME)
- Z. Bedőházi, Investigation of current in dielectrics induced by ultrashort laser pulses (Supervisor, P. Dombi, BME)
- V. Zsolczai, Optimization of nonlinear optical spontaneous parametric downconversion for quantum informational purposes (MSc, supervisor: Z. Kis)

Óbuda University, Budapest

- B. Leskó, Development of atomic beam probe diagnostics to COMPASS tokamak (BSc, supervisor: M. Palankai)
- Sz. Malik, Stability of muscle activities in human limb movements (BsC, Supervisor: J. Laczkó and Zs. Molnár*)

University of Szeged

- K.Bali, High intensity laser beam diagnostics (BSc, supervisor: I. Földes)

Ph.D students

Eötvös Loránd University, Budapest

- G. Balassa, Transport code cevelopment for heavy ion-simulations (Supervisor: Gy Wolf)
- D. Berényi, Theoretical investigations of the particle production in time-dependent strong fields at the LHC and ELI experiments (Supervisor: P. Lévai)
- G. Bíró, Investigation of particle production in high-energy heavy-ion collisions (Supervisors: G.G. Barnaföldi and G. Papp)
- Sz. Karsai, Investigation of the strongly-interacting matter in compact stars (Supervisors: G.G. Barnaföldi and E. Forgács-Dajka)
- P. Pósfay, Functional renormalization group method for the description of compact stars (Supervisors: G.G. Barnaföldi and A. Jakovác)
- M.F. Nagy-Egri, Numerical solutions of Einstein equations (Supervisor: I. Rácz)
- K.Z. Csukás, Initial value formulation of general relativity (Supervisor: I. Rácz)
- D. Barta, Dispersion of gravitational waves in interstellar media (Supervisor: M. Vasúth)
- G. Kasza, Search for new exact solutions of fireball fluiddynamics and interpretation of the measurement data of LHC and RHIC accelerators (Supervisor: T. Csörgő, co-supervisor: M. Csanád*)
- D. Kincses, Search for the critical point of strong interaction (Supervisor: M. Csanád (ELTE), co-supervisor: T. Csörgő)
- M. Lájer, Investigation of the String Field Theory vertex and boundary extensions of holographic dualities (supervisors Z. Bajnok and L. Palla)
- T. Gombor, Holography and the gauge gravity duality, (supervisor: Z. Bajnok)
- Gy. Bencédi, Identification of high-momentum particles with the ALICE detector at the LHC (Supervisor: P. Lévai, ELTE; Advisors: G.G. Barnaföldi, A.O. Velasquez [ICN/UNAM, Mexico City])
- O. Surányi, Study of the strong interaction with the CMS detector at the Large Hadron Collider (Supervisors: F. Siklér, G.I. Veres)
- É. Oláh, Particle physics teaching (Supervisors: D. Horváth, D. Varga)
- M. Novák, Design and construction of a high-field superconducting septum magnet for the Future Circular Collider (Supervisor: D. Barna)
- K. Brunner, Design and realization of an RF impedance measurement system at cryogenic temperature (Supervisor: D. Barna)
- M. Papp, Experimental and theoretical investigation of transitional-metal based functional molecules (Supervisor: G. Vankó)
- D. Réfy, Beam emission spectroscopy measurements to support understanding of H-mode of fusion plasmas (Supervisor: S. Zoletnik)
- M. Dósa, Space weather at the inner planets (Supervisors: G Erdős, K Szegő)
- A. Timár, Solar wind effects around a comet- investigations based on Rosetta measurements (Supervisor: Z. Németh)
- M. Máté, Studying strongly correlated systems using quantum information theory and tensor network state methods (Supervisors: Ö. Legeza, Sz. Szalay)
- Á. Vida, Preparation and investigation of multiphase high entropy alloys (Supervisor: L. K. Varga)
- P. Udvarhelyi, Ab initio calculation of magneto-optical parameters in solid-state qubits (Supervisor: Á. Gali)

- B. Korbuly, Phase-field modeling of complex polycrystalline patterns (Supervisor: L. Gránásy)
- L. Rátkai, Dynamics of crystalline self-organization within continuum theory (Supervisor: T. Pusztai)
- D. Datz, Chemical modification and near-field infrared microscopy of two-dimensional materials (Co-supervisor: Á. Pekker)
- S. Zsurzsa, Preparation and properties of nanowires (Supervisor: I. Bakonyi)
- V.A. Isnaini, Magnetic and magnetotransport properties of nanoscale ferromagnetic heterostructures (Supervisor: I. Bakonyi)
- P. Magyar, Response functions and collective excitations of strongly coupled plasmas
- (Supervisor: Z. Donkó)
- K. Bajnok, 5-7th century pottery production in transdanubia (Supervisors: L. Rosta, T. Vida* and Gy. Szakmány*)
- L. Kocsor, Preparation and characterization of rare-earth-doped crystals (Supervisors L. Péter and K. Sinkó*)
- É- Tichy-Rács, Synthesis, crystallization and spectroscopic investigation of rare-earth alkali borate scintillator materials (Supervisor: K. Lengyel)
- G. Kónya, Many-body physics in cavity QED (Supervisor P. Domokos)

Budapest University of Technology and Economics

- G. Nyitrai, High-performance muography (Supervisor: D. Varga)
- D. Szemes, Dynamics of light-activated functional molecules studied with ultrafast spectroscopy (Supervisor: G. Vankó)
- M. Lampert, Characterizing edge-plasma turbulence on the KSTAR tokamak with beam emission spectroscopy (Supervisor: S. Zoletnik)
- A. Buzás, Investigation of L-H transitions in fusion plasmas (Supervisor: A. Bencze)
- Ö. Asztalos, Beam emission spectroscopy diagnostics modelling (Supervisor: G. Pokol)
- G. Cseh, Investigation of transient processes in hot plasmas (Supervisor: G. Kocsis)
- D.R. Cserpán, Estimation of input signals based on multielectrode array measurements (Supervisor: Z. Somogyvári)
- P. Balla, Optical properties of magnetic materials (Supervisor: K. Penc)
- A. Csóré, Investigation of paramagnetic point defects in silicon carbide with atomic-level computational simulation (Supervisor: Á. Gali)
- Gy. Károlyházy, Controlled manufacturing of point defects in silicon carbide (Supervisor: Á. Gali)
- F. Podmaniczky, Dynamics of solidification, pattern and defect formation in phase-field crystal theories (Supervisor: L. Gránásy)
- G. Németh, Near-field infrared spectroscopy on two-dimensional systems (Supervisor: K. Kamarás)
- A.C. Cadena Nogales, Spectroscopic study of BN nanotube based hybrid nanostructure (Supervisor: K. Kamarás)
- M.D. Özeren, Photovoltaic study of perovskite-carbon nanocomposites (Supervisor: K. Kamarás)
- D. Nagy, Rheology of non-spherical granular particles (Supervisor: E. Somfai)
- T. Szarvas, Modeling of wave propagation and quantum optical processes in structured dielectrics (Supervisor: Z. Kis)

Al-Farabi Kazakh National University (Kazakhstan)

- U.U. Almasbek, The synthesis of composite nanoparticles and properties of the nanostructures formed in dusty plasma in electric discharges of different gas mixtures. The synthesis and properties of nanomaterials in complex gas-discharge plasma (Co-supervisor: P. Hartmann)
- R. Masheeva, Computer modeling and investigation of dusty plasmas in external electric and magnetic fields (Co-supervisor: Z. Donkó)

Jan Kochanowski University, Kielce, Poland

- M. Piotrovska, Study of conventional and non-conventional scalar and vector mesons, (Supervisors: P. Kovács and F. Giacosa*)

Óbuda University, Budapest

- D. Földes, Preparation and characterisation of new metal-organic frameworks (Supervisors: É. Kováts and S. Pekker)

Semmelweis University, Budapest

- E. Pálfi, Neural basis of the tactile perception in the somatosensory S1 area (Supervisor: L. Négyessy)
- Zs. Benkő, Causality analysis to reveal the dynamics, based on multichannel electrode measurements (Supervisor: Z. Somogyvári)
- Mir YM, Neural basis of tactile object perception in the SI somatosensory cortex. (Supervisor: L. Négyessy)
- N. Kiss, Application of nonlinear microscopy for investigation of skin tumours and rare genetic connective tissue disorders (Supervisors: N. Wikonkál* and R. Szipőcs)
- L. Fésüs, The effects of UV-light radiation on the physiological and pathological processes of the skin, on tumour development and its control mechanisms (Supervisors: N. Wikonkál* and R. Szipőcs)

University of Physical Education, Budapest

- P. Katona, The effect of kinematic parameters on the electrical activity of thigh muscles during cycling (Supervisor J. Laczkó)

Szent István University Gödöllő

- T. Baross, Hot isostatic pressing (HIP) welding in fusion relevant environment (Supervisor: G. Veres)

University of Debrecen

- J. Karancsi, Search for new particles with the CMS detector at the LHC (co-advisor: V. Veszprémi)

University of Pécs

- D. Jakab, Exotic phases and quantum phase transitions in many-body systems (Supervisors: G. Szirmai and Z. Zimborás)
- L.Á. Somlai, Study of rotating neutron stars (Supervisor: M. Vasúth)

- K. Varga-Umbrich, Study of coherent excitation and ionization of alkali atoms by strong laser pulses. (Supervisor: M.A. Kedves)
- M.A. Pocsai, Ab-initio quantum mechanical simulations to study photoionisation processes of rubidium atoms interacting with short and intense laser pulses (Supervisor: I. Barna)
- M. Mravcsik, Biological movement control and human-machine interface (Supervisor: J. Laczkó)
- L. Botzheim, Biological movement control and human-machine interface (Supervisor: J. Laczkó)
- I. Zsenák, Biomechanics of the adaptation of human limb movements to altered external physical environment (Supervisor: J. Laczkó)
- A. Walter, Studies on the moisture-dependent spread of injection agents for reinforcing construction materials (Supervisors: A. Len, A. Fülöp*)
- T. Steffgen, Experimental studies building physics investigations of condensation water on plaster surfaces (Supervisors: A. Len, A. Fülöp*)
- P. Körber, Proof of the effectiveness of water-repellent injection- methods for a subsequent masonry sealing, on the basis of experimental studies on bricks and mortar, using the scanning electron microscope in the ESEM- Mode, as well as in comparison with conventional detection methods (Supervisors: A. Len, E Sz Zoltán*)
- B. Bódi, Optimization of high harmonic generation (Supervisor: P. Dombi)
- V. Csajbók, Inducing ultrafast currents in dielectrics (Supervisor: P. Dombi)
- B. Nagy, Controlling photoelectrons on the nanoscale with plasmonic nanoparticles (Supervisor: P. Dombi)
- B. Lovász, Ultrafast photoemission from plasmonic nanostructures (Supervisor: P. Dombi)
- D. Jakab, Quantum phase transitions (Supervisor G. Szirmai)
- E. Molnár, Generating nonclassical states via coherent-state superpositions (Supervisor: P. Ádám)
- G. Mogyorósi, Generating nonclassical states in traveling optical fields (Supervisor: P. Ádám)
- F. Bódog, Optimization of periodic single-photon sources (Supervisor: P. Ádám)

University of Szeged

- Zs. Kovács, Investigation of ions from the Coulomb explosion of clusters and from the TNSA acceleration of thin solid targets (Supervisor I. Földes)
- Sz. Hack, Electrons in strong laser fields, attophysics. (Supervisors: S. Varró and A. Czirják*)
- I. Rigó, Synthesis and characterization of plasmonic nanostructures for surface enhanced Raman spectroscopic applications (Supervisor: M. Veres)
- M. Al-Lami, Investigation of neuron functions using stimulated Raman scattering (Supervisor: M. Veres)

Dissertations

Ph.D

M. Varga-Kőfaragó, Anomalous broadening of jet-peak shapes in Pb-Pb collisions and characterization of monolithic active pixel sensors for the ALICE inner tracking system upgrade (Supervisors: R. Snellings, J.F. Grosse-Oetringhaus, Utrecht University, Utrecht, The Nederlands)

É. Oláh, Particle phyiscs teaching at secondary schools (Supervisor: D. Varga, ELTE, 133 p.)

M. Aladi, High-order harmonics generation from noble gases clusters, (Supervisor I. Földes, PTE, 109 p. summa cum laude)

M. Lampert, Characterizing edge-plasma turbulence on the KSTAR tokamak with beam emission spectroscopy (Supervisor: S. Zoletnik, BME, 112p)

G. Thiering, First-principles study of diamond point defects (Supervisor: Á. Gali, BME, 174p)

T. Veres, Investigation of metal multilayers for neutron optics (Supervisors: L. Cser, L. Bottyán, ELTE, 104p)

A Szakál, Investigation of applications of atomic resolution neutron holography (Supervisor: L. Cser, BME, 111p)

Memberships

L. Almási
- Editorial Board of New Frontiers in Chemistry Journal (Timisoara, Romania)
- CANAM Scientific Selection Panel at NPI Rez, Czech Republic

A. Arató
- National contact of the Association for the Advancement of Assistive Technology in Europe (AAATE)
- Program committee member of the International Conference on Computers Helping People with Special Needs (ICCHP)

P. Ádám
- Laser Physics Committee of HAS.

K. Bajnok
- Geochemical, Petrographical and Mineralogical Scientific Board of the Archaeological Comission of the HAS

Z. Bajnok
- Particle Physics Committee of the HAS.
- Coordinator of the Gatis+ Network
- Physics Expert Panel of the Bolyai Fellowship

I. Bakonyi
- Solid State Physics Committee of the HAS (2011-2020)
- Editorial Advisory Board (2005-), Journal of Materials Science and Technology (Bulgaria, Sofia)
- European Board (2006-), European Academy of Surface Technology (EAST)
- EDNANO Board (2006-), International Workshop on Electrodeposited Nanostructures (EDNANO)
- Management Committee, COST MP 1407 action (2015-2019)
- Chairman (2017-2018), Award Selection Jury of "The Schwäbisch Gmünd Prize 2018" of EAST for Young Scientists
- Evaluation Committee (2018-2019), ITC Grant Applications, MPNS COST Action MP1407 "e-MINDS"

J. Balogh
- Int. Board on the Application of the Mössbauer Effect (IBAME), 2012-2018

J. Balog
- Particle Physics Committee of the HAS
- Chairman of the RMI Scientific Council

G.G. Barnaföldi
- Physics PhD School at Eötvös Loránd University, Budapest
- Hungarian representative, Board Member of the CERN LHC ALICE Collaboration,
- Group Leader of the Hungarian ALICE Group
- Hungarian representative, COST actions THOR CA15213 and PHAROS CA16214
- IAC member of the ISOTDAQ International School on Trigger and Data Acquisition
- IAC member of the International Conference series of the High-pT Physics for the RHIC/LHC Era

	—	General assembly of the HAS
	—	Wigner Intellectual Property Council
D. Barta	—	Virgo Scientific Collaboration
I. Bányász	—	Program Committee of Photoptics 2018 Conference
L. Bencs	—	Spectrochemical Work Committee of the HAS
	—	Work Committee for Environmental Chemistry of HAS
T.S. Biró	—	Chairman of the Zimányi Foundation for Physics
	—	Editor-in-Chief (theory) (2013-) of the European Physical Journal A: Hadrons and Nuclei (Springer)
	—	Editor of the Wigner Yearbook 2016-
	—	Physics PhD School, TU Budapest (BME)
	—	Physics PhD School, Eötvös University (ELTE) Budapest
	—	External member of the ELTE TTK PhD Council
	—	Nuclear Physics Committee at the HAS
	—	LOC member of the Zimányi School 2016-
	—	Presidential Publication Committee of the HAS
	—	Wigner Scientific Council (WTT)
	—	Natural Sciences Committee of the HAS, Chairman of the Physics 2 section
	—	Member of the Academia Europaea
L. Bottyán	—	Heinz Maier-Leibnitz Zentrum (MLZ) Review Panel Magnetism and Spectroscopy, Elastic Application
G. Böhm	—	Expert Panel W&T1: Mathematical Sciences, Fonds Wetenschappelijk Onderzoek – Vlaanderen (Scientific Research Fund – Flanders, 2012 -- 2018)
Á. Buka	—	Electronic-Liquid Crystal Communications, Editorial Board
	—	International Liquid Crystal Conference, International Advisory Board
	—	Solid State Physics Committee of HAS
L. Csernai	—	Editorial Board, International Journal of Modern Physics E - Nuclear Physics (World Scientific)
	—	Member of the Academia Europaea
	—	Member, Academia Europaea, Council
	—	Member of the Norvegian Scientific Academy
	—	Member of the Norvegian Academy for Technological Sciences
	—	External Member of HAS (2004-)
T. Csörgő	—	Chairman, International Advisory Committee, Zimányi Schools on Relativistic Heavy Ion Physics (2017-)
	—	Member of the Academia Europaea
	—	Section Committee, Physics and Engineering Sciences, Academia Europaea (2013-)
	—	Physics PhD School, ELTE, Budapest
	—	Institutional Board, PHENIX Experiment, BNL

- Executive Council, TOTEM Experiment, CERN LHC
- Editorial Board, TOTEM Experiment, CERN LHC
- CERN LHC Resource Review Board
- Principal Investigator, TOTEM - Hungary sub-collaboration
- Editorial Board, TOTEM experiment at CERN LHC
- Section Committee for Physics and Engineering Sciences, Academia Europaea (London)
- Professorial Council, Eszterházy Károly University
- IAC, Workshops on Particle Correlations and Femtoscopy (WPCF series)
- Diffraction and Low-x Conference Series (Regio Calabria, Italy), IAC member

A. Czitrovszky
- Chairman of the Laser Physics Committee of HAS
- President of the Hungarian Aerosol Society
- Chairman of the Hungarian EOS Chapter
- Chairman of the Optical Chapter of OPAKFI
- ELI-ALPS Scientific Advisory Committee
- Board of International Aerosol Association
- Board of European Arosol Assembly
- Representative of the Hungarian Aerosol Society at the Gesellschaft fur Aerosolforschung, Germany
- International Junge Award Committee
- Editorial Board of Fizikai Szemle

L. Diósi
- Management Committee of COST Action Quantum Technologies in Space CA15220

P. Dombi
- Commitee of Laser Physics of the HAS
- International Conference on Photonic, Electronic and Atomic Collisions, ICPEAC Program Committee
- Journal Editor at Scientific Reports (Nature Publishing)
- COST network "Nanospectroscopy", MC member
- Optical Society of America, senior member
- SPIE (Photonics Society), USA, senior member

P. Domokos
- Science and Engineering Board of the National Research, Development and Innovation Office
- Doctoral Council of the HAS
- Bolyai Scholarship Advisory Board of HAS
- Management Committee of COST Action MP1403 Nanoscale Quantum Optics
- Management Committee of COST Action CA16221 Quantum Technologies with Ultra-Cold Atoms
- Corresponding member of HAS (2013-)

Z. Donkó
- International Scientific Committee, Conference series "Symposium of the Phenomena in Ionized Gases" (2006-)
- International Advisory Board, Conference series "Strongly Coupled Coulomb Systems" (2007-)

	—	International Scientific Committee, Conference series "Symposium on Application of Plasma Processes" (2008-)
G. Dzsotjan	—	Committee of Laser Physics of the HAS
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	—	Deputy Chairman of the Committee on Astronomy and Space Physics of HAS
N. Éber	—	Editorial Board member of The Open Crystallography Journal (Bentham Open)
	—	Editorial Board member of the Journal of Research in Physics (DeGruyter)
	—	COST Action IC1208 MC member
P. Érdi	—	Board of Governors of the International Neural Network Society
	—	International Neural Network Society, senior member
	—	IEEE Computational Intelligence Society University Curriculum Subcommittee
G. Faigel	—	XFEL In-kind Review Committee
	—	XFEL SAC
	—	Member of the HAS
M. Fábián	—	ASTM International, Committee C26 on Nuclear Fuel Cycle
L. Fehér	—	International editorial board of Symmetry, Integrability and Geometry: Methods and Applications (SIGMA)
	—	International editorial board of Journal of Nonlinear Mathematical Physics (World Scientific)
P. Forgács	—	Particle Physics Committee of the HAS.
	—	Doctoral Council, Physics Section of the HAS.
	—	Doctoral Council, Doctoral School in Physics, Loránd Eötvös University
	—	Member of the General Assembly of the Astroparticle Physics European Consortium (APPEC)
I. Földes	—	Board member, EPS Plasma Physics Board, BPIF (Beam Plasma and Inertial Fusion).
J. Füzi	—	International Scientific Advisory Council of BNC (Budapest Neutron Centre)
	—	Editorial Board, Pollack Periodica
	—	International DENIM Committee
Á. Gali	—	Technical Program Committee (2011-), ICSCRM - International Conference on Silicon Carbide and Related Materials
	—	Technical Program Committee (2011-), ECSCRM - European Conference on Silicon Carbide and Related Materials

L. Gránásy	— ESA Topical Team "Solidification of Containerless Undercooled Melts", SOL – EML — Solid State Physics Committee of HAS — Mathematics and Science Committee of AKT — International Scientific Committee, SG18: 7th International Conference on Solidification and Gravity (Sept 3-6, 2018) Miskolc-Lillafüred, Hungary — Councillor representing Hungary in the International Organization for Crystal Growth (2016-2019) — Member of the Academia Europaea
D. Horváth	— Hungarian CERN Committee — Doctoral Council of the HAS — Editorial Board of Fizikai Szemle
F. Iglói	— Science Editor – Europhysics News — Editorial Board, European Physical Journal B — Statistical Physics Committee of the HAS. — Editorial Board of 'Fizikai Szemle' — International Advisory Board of the Middle European Cooperation in Statistical Physics (MECO) — Scientific Advisory Committee of the European Physical Journal
J. Janszky	— Laser Physics Committee of HAS — Member of the HAS
K. Kamarás	— Board of the Condensed Matter Division of the European Physical Society — Member of the HAS (2016-) — Member of the Academia Europaea
K. Kecskeméty	— Committee on Astronomy and Space Physics of HAS
Z. Kis	— Editorial Board of the Physical Review A
T. Kiss	— Commission on Quantum Electronics (C17) of the International Union of Pure and Applied Physics (IUPAP) — COST Action MP1006, MC member
G. Kocsis	— Nukleon Editorial Board — EUROfusion JET CDT2 Project Board — EUROfusion S1 Project Board
L. Kovács	— Hungarian National Committee, International Union of Crystallography — International Advisory Committee of EURODIM and ICDIM Conference series — Program Committee of the OMEE Conference series
P. Kovács	— General Assembly of the HAS
G. Kriza	— Solid State Physics Committee of HAS — Ph.D. School of Physics, BME

— Bolyai Fellowship Board, HAS
— Domus Hungarica Scientiarum et Artium Fellowship Board of the HAS

N. Kroó
— Chairman of the Governing Council of the Hungarian Research Infrastructure Program
— Chairman of the Rátz High School Prize
— Chairman of the Research Infrastructure Expert Group of ERA (EC)
— Chairman of Dennis Gabor International Prize Committee
— Hungarian UNESCO Committee
— High Level Expert Group on Digital Libraries and Scientific Publications (EC)
— Advisory Group on ESOF
— ELI_ALPS Scientific Advisory Committee
— Editorial Board, Laser Physics Letters (IOP Science)
— Member (former Chairman) of the Section of Physical and Engineering Sciences of Academia Europaea
— Member of the HAS

K. Kutasi
— International Scientific Committee, Conference series "International Workshop on Non-equilibrium Processes in Plasma Physics and Studies of Environment" (2006-)
— International Scientific Committee, Conference series of "Central European Symposium on Plasma Chemistry" (2013-)
— International Scientific Committee, Conference series "Europhysics Conference on the Atomic and Molecular Physics of Ionized Gases" (2015-)

J. Laczkó
— Society for Neuroscience
— International Society for Motor Control
— HAS Regional Committee in Pécs, Subcommittee of Mathematics and Informatics

A. László
— NA61 Collaboration Board

Ö. Legeza
— Statistical Physics Scientific Committee, HAS
— Young Researcher Committee, HAS
— Secretary of the Statistical Physics Section of Roland Eötvös Physical Society

P. Lévai
— Physics PhD. School, ELTE
— Hungarian CERN Committee
— CERN Council
— ESFRI (European Strategy Forum on Research Infrastructure)
— Committee on Research Infrastructure.
— Committee on Nuclear Physics.
— Committee on Particle Physics.
— International Association of Physics Students, honorary member
— Editorial Advisory Board of Journal of Non-Equilibrium Thermodynamics, de Gruyter

— Secretary of the Society for the Unity of Science and Technology
— the Accademia Peloritana dei Pericolanti (Classe di Scienze Fisiche, Matematiche e Naturali), corresponding member
— Member of the Academia Europaea
— Member of the HAS

B. Lukács
— Astronomical and Space Research Committee of the HAS.

F. Mezei
— Chairman of the European Physical Society Publication Committee
— Fellow of the American Physical Society (2000-)
— European Neutron Scattering Association (ENSA) Committee
— Scientific Advisory Council of SNS (Spallation Neutron Source), Oak Ridge National Laboratory, USA
— International Council for Scientific and Technical Information, University of California, San Diego, USA
— Member of the Academia Europaea, London
— Member of the HAS

A. Nagy
— Co-chairman of the Working Group Aerosol Measurement Technique in European Aerosol Assembly
— Scientific Program Committee of the European Aerosol Conference series

D.L. Nagy
— Common Coordination Committee of the HAS and the JINR, Dubna, HAS Representative
— Joint Institute for Nuclear Research, Dubna, Scientific Council
— Program Advisory Committee for Condensed Matter Physics, Joint Institute for Nuclear Research, Dubna
— European XFEL, Council
— FP7 Research Infrastructures Programme Committee, expert
— Chairman of the International Board of the Applications of the Mössbauer Effect
— European Synchrotron Radiation Facility, Consortium CENTRALSYNC, Steering Committee
— Hyperfine Interactions, Editorial Board
— International Union of Pure and Applied Physics (IUPAP), Commission on Physics for Development (C13)
— European Physical Society, Council
— European Strategy Forum on Research Infrastructures, Working Group on Regional Issues
— European Science Foundation, Organisation Forum on Research Infrastructures

Z. Németh
— Materials Science Work Committee of the HAS
— Work Committee on Nuclear Techniques for Structural Methods of the Chemistry Division of the HAS, president
— International Board on the Applications of the Mössbauer Effect
— Peer Review Committee (PRC4) for SOLEIL

É. Oláh	—	ELFT Board
A. Opitz	—	Guest editor of Journal of Space Weather and Space Climate: topical issue on 'Planetary Space Weather'
K. Penc	—	Solid State Physics Committee of the HAS
L. Péter	—	Secretary, EDNANO Board (2006-), International Workshop on Electrodeposited Nanostructures (EDNANO)
	—	Council of Graduate School of Chemistry, ELTE (2009-)
	—	Editor for Electrochemistry (Open Chemistry; formerly Central European Journal of Chemistry; DeGruyter, 2009-)
	—	Key Reader (Metallurgical and Materials Transactions E, Springer, 2014-)
	—	COST MP 1407 action, MC and training course coordinator, (2015-2019)
G. Pokol	—	Steering Committee of the ITER Core CXRS Consortium
	—	Project Board of the EUROfusion Work Package Code Development
	—	Vice-president of the Hungarian Nuclear Society
L. Rosta	—	Representative of the Eötvös Physical Society at the European Neutron Scattering Association
	—	European Spallation Source, Steering Committee
	—	Hungarian ESS Committee
F. Siklér	—	Institutional representative at the CMS Collaboration Board
	—	CMS Publication Committee, Heavy Ions editorial board
	—	CMS Management Board, as adviser to the Spokesman
	—	Particle Physics Scientific Committee of the HAS; Representative at the general assembly of the HAS; Member of the Nomination Committee of the HAS
	—	LHC Research Review Board (LHC RRB), Hungarian delegate
L. Somlai	—	Virgo Scientific Collaboration
	—	CREDO project
J. Sólyom	—	President of the Roland Eötvös Physical Society
	—	Member of the HAS
A. Sütő	—	Statistical Physics Committee of the HAS.
Zs. Sörlei	—	Committee of Laser Physics of the HAS
L. Szabados	—	Scientific advisory panel of the journal Classical and Quantum Gravity
	—	Particle Physics Committee of the HAS.
S. Szalai	—	Hungarian Space Research Council
	—	ARTEMIS-H steering
	—	Rosetta Lander steering
V. Szalay	—	CMST COST Action CM1405, MC member
Zs. Szaller	—	Thermoanalitical Committee of HAS

K. Szegő	—	Committee on Astronomy and Space Physics of HAS
	—	IAA
	—	ERC Starting Grant Evaluation Panel
E. Szilágyi	—	International Committee of the Conference series of Ion Beam Analysis
Z. Szőkefalvi-Nagy	—	Editorial Board, International Journal of PIXE (World Scientific)
	—	International Honorary Committee, PIXE
	—	Committee on Atomic and Molecular Physics and Spectroscopy, HAS
A. Telcs	—	Editor for Periodica Polytechnica (BME)
	—	Editor for Open Mathematics (De Gruyter)
Gy. Török	—	IAEA JRC-1575
	—	JRC-NET
B. Újfalussy	—	Secretary of the Materials Science Group of Roland Eötvös Physical society
	—	Executive Board of the Roland Eötvös Physical Society
	—	Secretary of the HAS Solid State Physics Committee
G. Vankó	—	Secretary of the Hungarian Synchrotron Committee, HAS
	—	EU COST Action MP1203 Advanced X-ray spatial and temporal metrology, MC member
	—	Hungarian representative in the European Synchrotron User Organisation
D. Varga	—	Particle Physics Scientific Committee of the HAS
L.K. Varga	—	International Organising Committee (2005-), International Conference on Soft Magnetic Materials (SMM)
	—	Advisory Committee (2004-), Czech and Slovak Conference on Magnetism (CSMAG)
M. Varga-Kőfaragó	—	ALICE junior representative
S.Varró	—	Commitee of Laser Physics of the HAS
	—	History of Science and Technology Committe of the H.A.S
M. Vasúth	—	Virgo Steering Committee
	—	PHAROS COST Action CA16214, MC member
	—	G2NET COST Action CA17137, MC member
P. Ván	—	Editorial board of Continuum Mechanics and Thermodynamics (Springer)
	—	Editorial Advisory Board, Journal of Non-Equilibrium Thermodynamics (De Gruyter)
	—	Secretary of the Society for the Unity of Science and Technology
	—	International Association of Physics Students, honorary member
	—	International Advisory Board, Zimányi Winter School series
	—	International Advisory Board, Joint European Thermodynamics Conference series

	— Corresponding member of the Accademia Peloritana dei Pericolanti (Classe di Scienze Fisiche, Matematiche e Naturali)
T. Vámi	— CMS Young Scientist Comitee, president
P. Vecsernyés	— Particle Physics Committee of the HAS.
G. Veres	— Governing Board, European Joint Undertaking for ITER and the development of Fusion Energy
V.Veszprémi	— CMS Management Board (ex officio) — CMS Tracker Institutional Board — CMS Tracker Management Board — CMS Phase 2 Tracker Upgrade Management Board — Advisory Committee of CERN Users
I. Vincze	— Doctoral Council of the HAS — Member of the HAS
A. Virosztek	— Solid State Physics Committee of the H.A.S.
G.Vizi	— Board member of the MANT (Hungarian Astronautical Society)
Gy. Wolf	— President of the International Theoretical Physics Workshop (NEFIM), Hungary — President of the of the Nuclear Physics Board, Roland Eötvös Physical Society — Leader of the Public Awareness of Nuclear Science (PANS) — Secretary of the Nuclear Physics Board of the HAS — Hungarian representative of the NuPECC EU FP7 HadronPhysics2, HadronPhysics3, HadronPhysicsHorizon, GSI FAIR, CBM, JRA Thuric, Toric, and Meson-Net projects. — Representative in Physics Department of the HAS — Nuclotron-based Ion Collider fAcility (NICA)
Z. Zimborás	— Editorial Board of Frontiers in Quantum Computing (Nature PG) — Editorial Board of PLoS ONE
S. Zoletnik	— Eurofusion/FuseNet panel to discuss PhD programmes of Baltic States — Eurofusion General Assembly — Eurofusion General Assembly Bureau — International Board of Advisors of the Institute of Plasma Physics, Prague — EURATOM Scientific and Technical Committe (STC) — Atomic and Molecular Physics Board of the HAS

Conferences

Workshop: "Introductory hands-on workshop on Tracker operations and DQM", 19-23 February 2018, LPC, Fermilab, Batavia, USA. — The workshop was organized by scientists from Wigner RCP, Inst. Nat. Phys. Nucl. et Particules Lyon, INFN Pisa, and the host institute, Fermi National Laboratory. The workshop took place in the LHC Physics Center in Fermilab, limited to 30 participants from six countries in order to be able to facilitate supervision for a set of hands-on sessions. It offered an introduction to the Pixel and Strips detectors, composing the heart of the CMS Tracker detector, including sessions on data-reconstruction, Tracker operations, and data quality monitoring.

Training course event of the COST MP 1407 program (Electrochemical processing methodologies and corrosion protection for device and systems miniaturization (e-MINDS)), Siófok, Hungary, 26-30 March 2018. — The e-MINDS training course is a unique training opportunity for young researchers from across Europe to get a complex insight into the interdisciplanary field comprising galvanotechnology, electrochemistry, corrosion, nanotechnology and materials science. The 2018 training course event had 74 students from 22 countries. The course event was organized to highlight 3 major topics: (i) Deposition of various materials: deposition chemistry and plating conditions, (ii) Organic functionalization of electrochemical systems, and (iii) Numerical simulations in electrochemistry. The main organizer was L. Péter as both the training course coordinator of the COST MP 1407 program and a local organizer.

12th Central European School on Neutron Techniques (CETS2018), Budapest, 6-11 May, 2018. — Budapest Neutron Centre (BNC – a consortium of HAS Wigner Research Centre for Physics and HAS Centre for Energy Research) hosted the 12th Central European Training School on neutron techniques. The objective of the school was to provide an insight into different neutron techniques: neutron scattering, imaging and elemental analysis, both at the level of tutorials as well as hands-on training.

This year 27 PhD students, postdocs, graduate students and young researchers attended the school. They arrived from 17 different European and non-European countries, with participants from Argentina to Korea and Tunisia to Israel. CETS2018 has taken a real global outreach. The organisers received nearly 50 applications this year, but the number of students by groups during the experimental work had to be restricted, thus attendees were selected with the above number.

Total 10 hours introductory lectures were given by renown experts from European neutron centres, such as ILL Grenoble, JINR Dubna, ESS Lund, University of Vienna as well as by BNC's leading researchers.

Total 15 hours (5 x 3) of practical work was offered to the participant groups: 5 persons groups were formed and rotated around 6 techniques using 8 instruments. The practical works were conducted by the local instrument scientists, the following type of experiments were available: wide angle and small angle diffraction instruments, reflectometer, prompt-gamma and neutron activation analysis stations and the neutron imaging facility.

On the opening day, the participants had the opportunity to present their work on posters and in the form of a flash oral presentation. On the last day, they received their well-earned certificates as well as special awards were given for the most active participants.

WPCF 2018, Cracow, Poland, 22-26 May 2018. — 88 participants, organized as members of the IAC

Workshop: The 672. WE-Heraeus Seminar "Search and Problem Solving by Random Walks", Physikzentrum Bad Honnef near Bonn (Germany) May 28 - June 1, 2018. — The main aim of the workshop was to discuss first detection/arrival problems for quantum and classical walks, for example, on a graph, and possible optimisation of search protocols. Better understanding parallels and fundamental differences between classical and quantum - in this particular context - will open the avenue towards solutions of many problems in the now emerging area of quantum information technology. The workshop served this goal by bringing together the two communities of scientists working on classical and quantum walks. There were around 80 participants from all over the world. Main orgainzer: Tamás Kiss, organizer: K. Penc)

Workshop "Mathematical Aspects of Spacetime Physics", Budapest, 29 May 2018, Budapest, Hungary. – The mini workshop was organized in order to discuss the Modugno theory of reference frame independent physics with the author. A possible collaboration between HAS Wigner RCP and University of Florence was also considered.

Workshop Support of Movement Rehabilitation by Functional Electrical Stimulation: current options and limitations in the interplay of advanced technology and physiological reality, 4 June 2018. — The workshop was organized by J. Laczkó (Wigner RCP) and W. Mayr (Medical University of Vienna. The workshop took place in in Prague, Czech Republik, as part of the World Congress on Medical Physics and Biomedical Engineering. Speakers of the workshop arrived from Austria, Germany, Hungary, Mexico, Spain and USA, and approx. 30 scientists participated at the workshop.

Conference "WE-Heraeus-Seminar: Trends in Quantum Magnetism", Bad Honnef, 4-8 June 2018. — Magnetism is an old subject: the material magnetite has been known for thousands of years. Yet, the richness of magnetic materials and phenomena continues to fascinate us with new ideas, problems, and concepts. The description of the interacting spins in magnetic insulators is a major challenge for theory, and the precise understanding involves ingenious theoretical tools and advanced numerical methods, like tensor networks and Monte-Carlo methods. Recently, concepts of topology are being used increasingly also in the field of magnetism to describe states and excitations in materials. The ideas developed for magnetic Mott insulators are also applied to cold atoms in optical lattices, a new fast growing field of physics.

Conference PallaFest, Celebrating the 70th birthday of László Palla, 14-15 June 2018. — The international conference was organized to celebrate the 70th birthday of our colleague, László Palla and discuss ideas in the field of two-dimensional integrable models. We had 14 talks and more than 30 participants from all over the world.

Symposium: "Quantum electronics 2018: 8th Symposium on Hungarian Quantum Electronics Research", Budapest, 15 June 2018. — The symposium was organized by the Atomic and Molecular Physics and Quantum Electronics Group of the Roland Eötvös Physical Society, the

Committee on Laser Physics and Spectroscopy of the Hungarian Academy of Sciences, and the Institute of Physics of the Budapest University of Technology. The symposium took place in Building “K” of the Budapest University of Technology. The aim of the symposium was to review the results of the researches conducted in Hungary in the fields of optics, atomic and molecular physics and plasma physics. Scientists participating in the symposium represented seven Hungarian institutes, they could attend nine presentations and get acquainted with the findings of other groups on 54 posters.

Workshop “8th GPU Day, The Future of Computing, Graphics and Data Analysis”, 21-22 June 2018, Wigner RCP, Budapest, Hungary. — The “GPU Day” series has been organized by the Wigner GPU Laboratory for the 8th times in this year. The two-day workshop interconnects scientists, programmers, and parallel-computing experts from all over the world. This year we had 80 participants and visitors from Germany, CERN, Poland, UK. Several commercial companies visited the event from Hungary and abroad. Relevant support was received from Lombiq LTD and EPAM Systems LTD.

GPU-Day, “The Future of Many-Core Computing in Science”, Budapest, 21-22 June 2018. — The 8th in the conference series organized by the Wigner Research Centre for Physics of the Hungarian Academy of Sciences is dedicated to the field of many-core computing in scientific and industrial applications. Topics include: Current status and near-future of parallel and high-performance hardware and software, Many-core computing in physics and other fields of science, Medical applications of parallel technologies, Graphics, rendering and image synthesis, Machine Learning, Neural Networks, feature recognition, Image processing, computer vision and reconstruction, Industrial applications, Quantum computing, Mobile and embedded computing, Emerging accelerator platforms, Development technologies (languages, compilers, tools).

CECAM Workshop: Crystal defects for qubits, single photon emitters and nanosensors, Bremen, Germany, 9-13 July 2018. — The scientific objectives of the proposed workshop are to bring together researchers from materials growth, defect engineering, surface chemistry, quantum optics, spin physics and theory at phenomenological and atomic scale level to highlight recent progress and discuss challenges and opportunities in the host materials and the embedded defects from the aspect of realization and control of quantum bits for quantum information processing and sensing; as well as to discuss possibilities for optimizing the materials properties and device design aided by theory. The interdisciplinary character of the workshop helps finding solutions for overcoming current limitations.

https://www.cecam.org/workshop-1561.html

11. BerzeTÖK Science, 9-13 July 2018, Mátraszentimre, Hungary. — (5 days, 36 science outreach talks, T. Csörgő chair and organizer, speakers included T. Csörgő and G. Kasza); https://indico.kfki.hu/event/863/ Eight talks were given by speakers with Wigner affiliation. Our group leader is regularly organizing Science Summer Camps as social events. Typically, these are attended by about 25 secondary school students predominantly from the Berze Secondary Grammar School of Gyöngyös, Hungary. These events are open for nearby primary and secondary school students, their teachers as well as their parents and senior citizens.

Diffraction and Low-x 2018 Meeting, Reggio Calabria, Italy, 26 August – 1 September 2018. — 82 participants, organized as members of the IAC

Conference „Quantum Magnetism: Frustration, Low-dimensionality, Topology", Kavli Institute for Theoretical Sciences & IOP-CAS Workshop, Beijing, China, 27 August – 14 September 2018. — Organizers: Frederic Mila (Lausanne, Switzerland), Gang Chen (Shanghai, China), Karlo Penc (Budapest, Hungary), Xiaoqun Wang (Shanghai, China), Tao Xiang (Beijing, China)

European Conference on Silicon Carbide and Related Materials, Birmingham, UK, 2-6 September 2018. — The European Conference on Silicon Carbide and Related Materials (ECSCRM) is a highly-anticipated event, held every two years, that represents an important international forum that brings together world-leading specialists working in different areas of wide-bandgap semiconductors. Experienced researchers, experts from leading companies (40 in total) and young students interested in this specific scientific domain exchange their views and ideas in 11 subtopics of the subject. (> 700 attendees)

Seventh International Conference on Solidification and Gravity (SG'18), 3-6 September 2018, Miskolc – Lillafüred, Hungary.

https://warwick.ac.uk/fac/sci/eng/ecscrm2018/

ELFT Summer School Astroparticle Physics, Mátraháza,3-7 September 2018. — In 2018 the ELFT Summer School organized by Zsolt Szép (ELTE) and Zoltán Zimborás (Wigner RCP) took place at the Mátraháza Holiday Resort of the Hungarian Academy of Sciences in the first week of September. The theme of the Summer School was Astroparticle physics, which is a quickly developing interdisciplinary research field that lies at the intersection of particle physics, cosmology, and astrophysics. This field tries to answer some of the basic questions about the Universe by experiments and observations that merge the capabilities of the advanced detectors of particle physicists with the highest standard of imaging of the cosmos undertaken by astrophysicist. The following topics were covered: Dark Matter and Dark Energy, Particles in and from Space, Gravitational Waves and Multi-messenger Observations.

ISMD 2018, Singapore, 3-7 September 2018. — 117 participants, organized as members of the IAC

European Materials Research Society Fall Meeting 2018, symposium O (Diamond for electronic devices III), Warsaw, Poland, 17-20 September 2018. — The meeting follows the successful symposia held in 2016 and 2017 with an update on progress in the field. Several topics are of particular interest, although papers on all aspects of diamond technology are welcome. These include diamond for power electronics, diamond nano-electronic devices, diamond for quantum applications and diamond for bio-devices. In all cases, man-made single crystalline diamond is used either as ultra-pure layer or semiconducting by boron and phosphorus doping. The growth and deposition of high quality diamond films are therefore a subtopic at the symposium. Quantum metrology applications (for example, magnetrometry based on NV centres) is of key interest.

https://www.european-mrs.com/diamond-electronic-devices-iii-emrs

Workshop "CREDO workshop and educational event Budapest 2018" 20-21 of September 2018 Hungarian Academy of Sciences (Wigner RCP), Budapest, Hungary. — The Cosmic-Ray Extremely Distributed Observatory (CREDO) Budapest event was organized by the Institute of Nuclear Physics, Wigner Research Centre of Physics. The workshop and educational event are dedicated to ensembles of cosmic rays: yet unseen messengers of the Universe. We had 40 participants.

Conference "The first 30 years of Reverse Monte Carlo Modelling" Budapest, Hungary 20-22 September 2018. — The 7th Reverse Monte Carlo conference was organized by the members of the Liquid Structure group. The conference took place in Hotel Holiday Beach, Budapest. Besides scientists from Hungary, guests arrived from the USA, UK, Japan, Slovakia, Latvia, Italy, Germany and France. The three-day meeting which was attended by approx. 65 scientists boosted the cooperation between researchers of materials science and solid state physics.

Conference "Entanglement Days 2018", Budapest, 26-28 September 2018. — The international conference was organized by Géza Tóth, Zoltán Zimborás, Szilárd Szalay, and János Asbóth, all of them researchers of Wigner Research Centre for Physics, on theoretical questions related to quantum entanglement, a central topic in foundations of quantum physics, and an important resource in quantum information processing and quantum metrology. The conference funded by the University of Basque Country and the Wigner Research Centre took place at the Budapest University of Technology and Economics (building A), lasted three days, with invited talks from internationally acclaimed researchers, contributed talks, as well as two posters sessions, where the participants could discuss their results. Of the 81 participants, around 20% were Hungarians, and so the conference gave also an opportunity for local researchers and students to get a glimpse of the status of this field.

Entanglement Days 2018, Budapest, 26-28 September 2018. — International conference, 100 registrated participants.

Workshop „Tailoring Light-Matter-Charge-Interactions in Polar-Oxide Nano-Architectures", Budapest, Hungary, 6 October 2018. — The workshop was organized as a preparatory meeting for the submission of the „oXtronics" proposal (Tailoring Light-Matter-Charge-Interactions in Polar-Oxide Nano-Architectures) to the EU COST program. (6 participants)

Planck 2018 Memorial Scientific Symposium, Budapest, 10-11 October 2018. — The "Planck 2018 Memorial Scientific Symposium" was organized on the occasion of Max Planck's 160th birthday and of the 100th anniversary of his receiving the Nobel Prize in Physics. The conference took place in the main building of the Hungarian Academy of Sciences, and organized by the Committee on Laser Physics and the Joint Committee on History of Science and Technology (Chairmen: S. Varró, M. Bonitz and B. Láng). The number of registered participants were more than 100. At this two-day memorial scientific symposium there were only plenary talks on each day delivered by leading experts. They discussed historical aspects, Max Planck's contribution to physics, and some present scientific challenges.

Conference: HEPTECH AIME ML&VA on Clouds, 29-30 October, Hotel Mercure, Budapest, Hungary. — The aim of this event is to bring together Academic researchers and Industry experts to share ideas, potential applications and fostering collaborations in the newly emerging field of Machine Learning and Visual Analytics and related technologies. Topics of the workshop include: machine learning, artificial Intelligence, Big Data, visual analytics, quality of life, computational neuroscience, computational linguistics, computational physics, cloud computing technology, data quality, data security. We had 88 participants and several industrial partners.

4th Day of Femtoscopy, Eszterházy Károly University, Gyöngyös, 30 October, 2018. — 21 participants, 21 talks.

Workshop "Lectures on Modern Scientific Programming", 20-21 November 2018, Wigner FK, Budapest, Hungary. — This international workshop of the Wigner GPU Laboratory is dedicated to widen our knowledge and practice on parallel computing in science. The seminar-series-like event started from the basics of artificial intelligence, then moved to practical deep neural network programming techniques for physicists. We had 60 registered participants mostly from the Hungarian and abroad universities.

Symposium in Memoriam Zoltán Gyulai, Budapest, Hungary, 15 November 2018. — A symposium has been organized at the Institute for Solid State Physics and Optics dedicated to the memory of Zoltán Gyulai (1887-1968), the father of Gyulai-Tarján Crystal Physics School. (10 lectures)

Inaugural Presentations by New Members of Academia Europaea in Barcelona, Spain, 28 November, 2018. — 12 presentations, co-chaired with Professor M. Harakeh

Conference "Zimányi Winter School '18": 18th Zimányi Winter School on Heavy Ion Physics", 3-7 December 2018, Budapest, Hungary. — This traditional one-week international winter school is organized jointly by the Eötvös University and the Wigner RCP dedicated for József Zimányi, the founder-father of the Hungarian High-energy Heavy-ion school. In this year we have organized this event for the 18th time, providing an excited platform for discussion between students and world-class experts of the high-energy heavy-ion collisions both form theoretical and experimental sides. We had about 100 participants including visitors from the US, China, Mexico and European countries, representing the huge experimental collaborations, such as ALICE, CMS, LHCb from CERN, Switzerland besides STAR and PHENIX from the BNL, USA. Contributions will be edited in a conference proceedings in PoS.

18th Zimányi Winter School and Workshop on Relativistic Heavy Ion Physics, Budapest, 7-12 December 2018. — In collaboration between Wigner RCP, Eötvös L. University and Eszterházy K. University, 5 days, 85 talks, 104 participants, including 35 PhD students.

Czitrovszky Aladár: Symposium on Medical Applications of Lasers, Lasram Ltd.

Wigner Colloquia

In the fall of 2014 we started to organize a series of Wigner Colloquia, inviting international experts to deliver talks on fresh and interesting research topics to the entire community of our research centre. We also have dispatched a modest financial background to support this activity by occasionally reimbursing travel costs to and accommodation costs in Budapest for the invited speakers.

The concept of this series is to offer to our researchers a possibility to meet colleagues from external institutions who work on hot topics and able to present their favorite research to a wide audience of physicists, working both in experiment and theory in fields ranging from high-energy particle physics via nuclear and plasma physics to materials and life science related problems. We restrict our invitations in number to a few per semiannual blocks.

Wigner Colloquia in 2018

https://indico.kfki.hu/category/42/

27-03-2018	Xu-Guang Huang, Anomalous chiral transport phenomena in heavy-ion collisions
24-04-2018	Marko Robnik, "Quantum chaos of generic systems: Divided phase space, localization of chaotic eigenstates and spectral statistics"
08-05-2018	May Reinhard Alkofer, "Electron-Positron Pair Production in Laser Fields"
02-10-2018	Chi Keung Chan, "Anticipating Dynamics of Retina"
13-11-2018	Berndt Müller, "The Unbearable Burden of Being Light: Exploring the emergence of ordinary matter from quarks and gluons"
04-12-2018	Chihiro Sasaki, "Phases of Quantum Chromodynamics at Extremes"

Seminars

Weekly meetings of the Budapest and Debrecen Compact Muon Solenoid (CMS) groups:
https://indico.cern.ch/category/8677/

Wigner RCP RMI Seminars

Theoretical physics seminars

http://indico.kfki.hu/category/28/

26 01-2018	Gy. Wolf (Wigner RMI): Charmonium $(\bar c c)$ mass in antiproton-nucleus reactions, how the in-medium gluon condensate can be measured
02 02-2018	C. Ahn (Ewha University, Seoul): Giant magnon-like solution in Sch5 x S5
05 02-2018	M. Piotrowska (Jan Kochanowski University, Kielce): Testing the quark-antiquark picture in the light meson sector
09 02-2018	F. Giacosa (Jan Kochanowski University, Kielce): Aspects of non-exponential decay
16 02-2018	D. Horváth (Wigner RMI): Muons: what are they good for?
23 02-2018	Z. Kökényesi (Wigner RMI): Chiral expansion and Macdonald deformation of two-dimensional Yang-Mills theory
02 03-2018	H. Feichtinger (Univeristy of Vienna): A function space defined by the Wigner transform and its Applications
09-03-2018	Y. Jiang (ETH): Algebraic geometry and Bethe ansatz
23-03-2018	B. Koczor (TU München): Continuous phase-space representations for finite-dimensional quantum states and their tomography
27-03-2018	A. Bhattacharyya (University of Calcutta): Fluctuations and Correlations in Heavy Ion Collisions
06-04-2018	A. Sütő (Wigner SZFI): Phase transitions in homogeneous systems of interacting bosons
13-04-2018	O. Kálmán (Wigner SZFI): Measurement-induced nonlinear transformations for quantum information processing tasks
27-04-2018	K. Shen (Heavy-Ion Wigner Research Group) : Investigations on the Quantum Statistics in Non-extensive Physics and its Phenomenological Applications in High-energy Nuclear Physics
04-05-2018	T. Wang (Lanzhou University): Introduction of the Nuclear Research Activities in Lanzhou, China
11-05-2018	E. Hatefi : Universality in string theory
25-05-2018	M. Gyulassy (Prof. emeritus, Wigner RCP, Columbia University): Precision Dijet Acoplanarity Tomography of the Chromo Structure of Perfect QCD Fluids
28-05-2018	M. Modugno (Florence): Covariant Quantum Mechanics
31-05-2018	I. Bautista Guzman (BUAP, Puebla, Mexico & CERN ALICE): Collectivity in small collision systems how far is it from the thermodynamic phase transition
01-06-2018	Z. Keresztes (Univ. Szeged) : Spin evolution of compact binaries from post-Newtonian secular dynamics
04-06-2018	Ashik Ikbal Sheikh (Kolkata India): Taking a walk with heavy quarks in a field fluctuating Quark-Gluon Plasma at the LHC energies

19-06-2018	J. Rafelski : Quantum Vacuum and Strong Fields
03-08-2018	F. Krizek(Alice): Hadron+jet correlations in ALICE
13-08-2018	D. Molnár (Purdue University): Self-consistent viscous phase space distributions from kinetic theory
27-08-2018	S. Simic (Novi Sad): Multi-temperature mixtures of gases
21-09-2018	S. Abe (Mie University, Japan): Estimating Entanglement
23-11-2018	L. Diósi (Wigner RMI): Quantum control and semiclassical quantum gravity
26-11-2018	Gy.P. Gehér (University of Reading): Wigner's theorem on quantum mechanical symmetry transformations
30-11-2018	V. Procházka (Uppsala University): Boundary CFTs and their central charges

Wigner Space Seminar

http://www.rmki.kfki.hu/~opitz/WignerSpaceSeminar

22-03-2018	Zeldovich M.A., Logachev Yu.I., Kecskeméty K., Quiet-time 0.04 – 2 MeV/nucleon Ions at 1 AU in Solar Cycles 23 and 24, Solar Physics (in press): DOI 10.1007/s11207-017-1170-8.
26-10-2018	Mercure and the BepiColombo programme. Review of the details of BepiColombo programme, with the prospective results. Launch is planned on 20 October 2018

Wigner RCP SZFI Seminars

https://www.szfki.hu/seminar

04-01-2018	B. Náfrádi (EPFL Lausanne): Magnetic-photoconductors: A versatile platform for light controlled magnetism
09-01-2018	B. Dóra (BUTE Department of Theoretical Physics): Momentum space entanglement in Luttinger liquids
30-01-2018	T. Veres (Wigner RCP SZFI): Examination of metal thin films for neutronoptics (in-house thesis defence)
30-01-2018	Ch. Schilling (Clarendon Laboratory, University of Oxford, UK): Universal upper bounds on the Bose-Einstein condensate
06-02-2018	P. Pyshkin (Wigner RCP SZFI): How to speed up holonomic quantum computation: net zero-energy-cost control in decoherence-free subspace
13-02-2018	S. Tóth (Wigner RCP SZFI): Preparation of nanocrystals by femtosecond laser pulses
20-02-2018	L. Oroszlány (Faculty of Physics of Complex Sysytems, ELTE): A new class of topological materials: nodal line semimetals
06-03-2018	M. Tegze (Wigner RCP SZFI): X-ray scattering on individual particles by free-electron laser
13-03-2018	L. Rátkai (Wigner RCP SZFI): Phase-field modeling of spiral euthectic dendrites (in-house thesis defence)
27-03-2018	Z. Horváth (Wigner RCP SZFI): KFKI Anno (View from under)
03-04-2018	Á. Lukács (TU Delft): Weyl discs
10-04-2018	T. Szarvas (BUTE, Department of Atomic Physics): Simulation of electromagnetic wave propagation in structured dielectrics

12-04-2018	Hamed Merdji (Service des Photons Atomes et Molécules, CEA Saclay, France): High harmonic generation in 2D and 3D semiconductors
17-04-2018	B. Korbuly (Wigner RCP SZFI): Description of polycrystalline solidification forms and grain coarsening in the frame of phase-field theory (in-house thesis defence)
19-04-2018	A. Ganin (School of Chemistry, University of Glasgow, UK): Activating the basal plane of a 2D chalcogenide for electrocatalytic hydrogen evolution reactions
24-04-2018	I. Pethes (Wigner RCP SZFI): Unordered ordered systems
03-05-2018	T. O'Brien (Leiden University): Quantum error correction for near-term devices
08-05-2018	B. Hetényi (Department of Physics, BUTE and Bilkent University, Turkey): Berry phases and topological physics in one-dimensional systems
15-05-2018	S. Varró (Wigner RCP SZFI): Black-body radiation and the forgotten heritage of Max Planck
22-05-2018	D. Földes (Wigner RCP SZFI): Preparation and characterisation of new metal-organic frameworks
29-05-2018	Gy. Faigel (Wigner RCP SZFI): Structure determination from one laser pulse
31-05-2018	Gy. Károlyházy (Wigner RCP SZFI): Controlled preparation of point defects in silicon carbide (work summary)
05-06-2018	D. Beke (Wigner RCP SZFI): Preparation of very small silicon carbide nanocrystals for teranostic and quantum technology applications
05-06-2018	É. Tichy-Rács (Wigner RCP SZFI): Single cristals as photon sources of quantum technology (work summary)
12-06-2018	A. Majumdar (Dept of Mathematical Sciences, University of Bath, UK): Multistability in confined nematic systems: analytical and numerical approaches
19-06-2018	G. Thiering (Wigner RCP SZFI): First-principles calculation of diamond point defects (in-house thesis defence)
26-06-2018	M. Ford (University of Technology Sydney, and Flinders University of South Australia): Designing novel hybrid materials from two-dimensional building blocks
03-07-2018	P. Thunier (CERN): Detectors and electronics for neutron detection at the NMX instrument of the European Spallation Source ERIC (ESS)
04-09-2018	P. Dombi (Wigner RCP SZFI): Ultrafast physical experiments in the collaboration of Wigner RCP and ELI-ALPS
11-09-2018	L. Péter (Wigner RCP SZFI): Materials testing possibilities on the new scanning electron microscope of the Wigner SZFI
13-09-2018	B. Náfrádi (Laboratory of Physics of Complex Matter, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland): Hybrid halide perovskite: A game changer for telecommunication?
18-09-2018	P. Schneeweiss (Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien): Two quantum optics experiments in extreme parameter regimes
25-09-2018	V. Ivády (Wigner RCP SZFI and Linköping University, Sweden): New approaches for spin dynamic simulations of point defect qubits

09-10-2018	Gy. Faigel (Wigner RCP SZFI): Scientific performance of Wigner RCP SZFI/SZFKI of the HAS in the last twenty years
16-10-2018	U. Wolff (Leibniz Institute for Solid State and Materials Research, Institute for Metallic Materials, Dresden, Germany): In-situ observation of the reversible electrochemical deposition of Fe in transmission electron microscopy
29-10-2018	R. Stannarius (Dept. of Nonlinear Phenomena, Otto von Guericke Uni Magdeburg): Granular gases
30-10-2018	K. Penc (Wigner RCP SZFI): Topological magnons in Kitaev magnets at high fields
06-11-2018	L. Vitos (Wigner RCP SZFI): Plasticity of austenitic steels from quantum mechanical modeling
13-11-2018	A. Mallick (Wigner RCP SZFI): Discrete quantum walk simulation of neutrino oscillation and Dirac particle dynamics in curved space-time
20-11-2018	A. Vukics (Wigner RCP SZFI): Of atomic clocks
27-11-2018	Z. Erdélyi (Faculty of Natural Sciences and Technology, Univ. Debrecen): Two-component metal and porous metal/metal oxide nanoparticles
04-12-2018	I. Földes (Wigner RCP RMI): High harmonics and spectral interferometry, isolated attosecond pulses from solid state laser plasmas
11-12-2018	R. Stannarius (Dept. of Nonlinear Phenomena, Otto von Guericke Uni Magdeburg): Granular gases
18-12-2018	P. Dombi and P. Domokos (Wigner RCP SZFI): The Nobel Prize in Physics 2018