

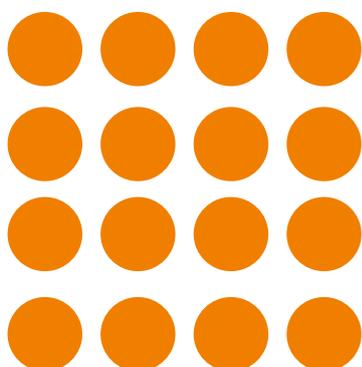


UNIVERSITY  
OF WARSAW



University of Warsaw  
Biological and Chemical  
Research Centre

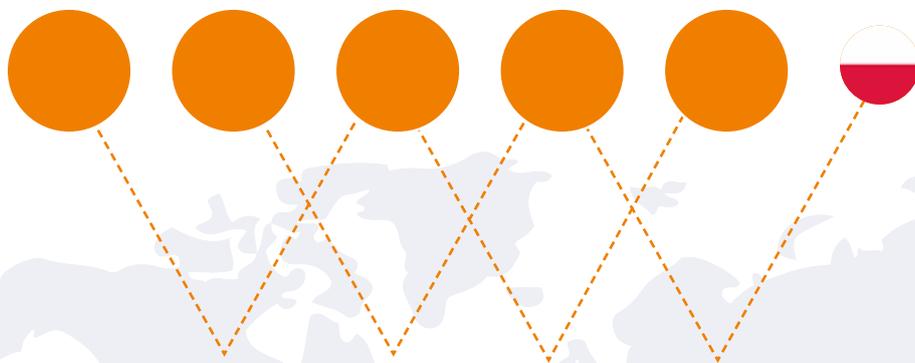
**VISITING  
PROFESSOR  
PROGRAMME**



**two editions** 1.09.2018-30.09.2020  
**16 visiting professors**

FROM

**5 continents**



also  
**Polish scientists  
with international  
successes**

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# VISITING PROFESSOR PROGRAMME

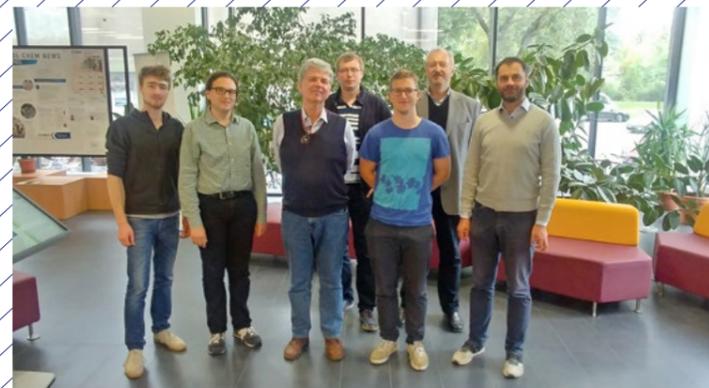


Photo gallery

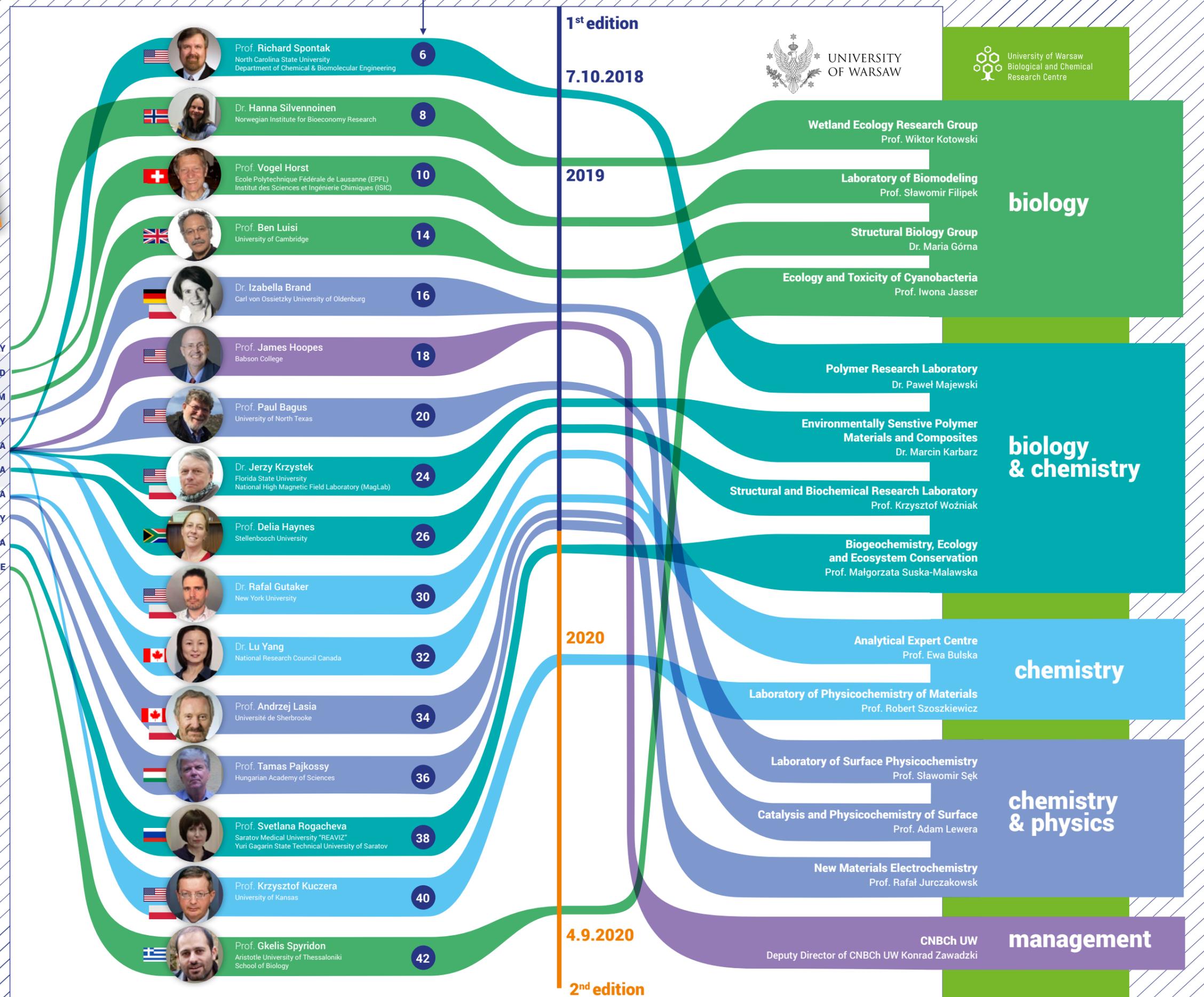
The Visiting Professors Programme was dedicated to outstanding scientists working outside of Poland. The purpose of the programme was to strengthen the international profile and competitiveness of the University by increasing the proportion of international researchers, and to build deeper relationships with a number of reputable universities and schools around the world.

We hosted sixteen visiting professors from five continents who contributed in many different ways in both research and education. CNBCh UW scientists had a possibility to attend in interesting public lectures and seminars. Professors were also involved in projects implemented by researchers from our Centre. The project had its own visual identity, including a logo, new website. Applications of candidates took place online. All promotional material were in compliance with this graphic. From the moment of registration, we were in contact with scientists and we were honored that we could meet all the outstanding scientists from different part of the globe. Thanks to the involvement of many people, the program was very well received and enjoyed great popular .

**VISITING PROFESSOR PROGRAMME**

page number

- NORWAY
- SWITZERLAND
- UNITED KINGDOM
- GERMANY
- USA
- SOUTH AFRICA
- CANADA
- HUNGARY
- RUSSIA
- GREECE



**16 visiting professors**  
 FROM **10 countries**  
**5 continents**  
 VISITED **13 laboratories**  
 DELIVERED **22 lectures**



University of Warsaw  
Biological and Chemical  
Research Centre

**biology**

**biology & chemistry**

**chemistry**

**chemistry & physics**

**management**



CNBCh Research Group:  
**Polymer Research Laboratory**  
headed by Dr. Paweł Majewski

## Prof. Richard Spontak

### Activity at Home University:

Prof. Spontak's research interests include effects of homo/copolymer blending, molecular architecture, monomer sequencing, and solvation on the phase behavior of microstructural polymer systems.

### Activity at CNBCh UW:

Prof. Spontak was a consultant of the project „Innovative Nanostructured Functional Materials by Combinatorial Methods of Directed Self-Assembly of Block Copolymers”. Prof. Spontak also delivered a series of lectures for students at the UW Faculty of Chemistry and seminars.

**University:** [North Carolina State University](#)

**Country:** USA, Raleigh

**Date of stay:**  
7–21 October 2018

### Dr. Paweł Majewski about cooperation

Prof. Spontak delivered two research seminars during his stay at the Center. On 10/08/2018 he gave a talk *Directed Self-Assembly of Block Copolymers as a Route to Novel Hierarchical Superstructures* dedicated for graduate students and faculty members of the Department of Chemistry of UW. On 10/25/2018 he delivered an interdisciplinary research seminar for biologists and chemists employed at the Center focused on the role of self-sterilizing materials in the fight against antibiotic-resistant pathogens, *Photodynamic Polymers as Comprehensive Self-Sterilizing Materials: Staying Ahead of a Growing Global Threat*. Collaboration between the UW and NCSU: Professor met individually with the Dean of Chemistry Department - Prof. Andrzej Kudelski and with the Director of the Center, Prof. Ewa Bulska. Since NCSU is, similarly to the UW a public school, challenges of securing funding from grants and training graduate students were discussed. Also, RS described a way in which the graduate school already operates at NCSU, and which will soon be introduced at the UW. In the discussion with Prof. Bulska, he shared some ideas on how to encourage graduate students working at the Center to more frequently attend research seminar organized by the Center. Teaching: Professor taught a short course in polymer science -Recent Advances in the Design and Characterization of Polymer Systems Based on Block Copolymers. The course consisted of four meetings, two teaching-units each and was attended by 12 students (9 from the UW and 3 from the Warsaw Polytechnics). His last lecture was specially dedicated for the EM microscopists working at the Center. 1st lecture: The Phase Behavior of Polymer Blends and Block Copolymers 2nd lecture: Rethinking Responsive Soft Elastomers from Com-

position-Tunable Thermoplastic Elastomer Gels. 3rd lecture: Controlling the Phase Behavior of Model Block Ionomers for Contemporary Technologies 4th lecture: Applications of Advanced Electron Microscopy in Polymer Science The students, who attended a course and submitted take-home exams, which were graded were credited with 2 ECST points counting towards the required PhD course-load. Research and advisory role: I was meeting with RS daily during his stay and engaged him in daily research activities of my group. We have primarily discussed scientific progress in my First Team project and consulted future research directions. I have also received a handful of insightful comments regarding the organization of work in my group. Professor attended our weekly research meetings and gave feedback on presentations by our PhD and MSc students. They also had multiple opportunities to ask him science-related questions.

Results of the visit: The results of the visit are two-fold: daily interactions with an established scientist and attending his lectures helped me and my group to find a broader perspective for our research. Research-wise, we have established a collaboration between his and our group in TEM tomography (one of the areas of his core-expertise). He gave us detailed instructions on sample preparation including technical details of staining and handling the block-copolymer samples. We will send some of the materials produced in our lab to his group for T-TEM investigations. The students have benefitted by attending seminars and lecture series given by the world-class researcher and talented academic teacher.

# LECTURE

## Prof. Richard Spontak

North Carolina State University

### Photodynamic Polymers as Comprehensive Self-Sterilizing Materials: Staying Ahead of a Growing Global Threat

**DATE:** 5 October 2018 |15:00.

**VENUE:** CNBCh UW, Hall B

#### ABSTRACT:

Adherence of pathogens such as bacteria and viruses on various surfaces routinely leads to subsequent transmission to new hosts, significantly promoting the proliferation of potentially harmful organisms. This sequence is particularly worrisome in the case of antibiotic-resistant pathogens, which are becoming a global threat to human health. According to the Centers for Disease Control and Prevention, 1 out of every 20 hospital patients is affected by nosocomial infections, subsequently resulting in 100,000 deaths annually in the United States alone. Out of these, about 23,000 deaths are attributed to drug-resistant pathogens such as methicillin-resistant *Staphylococcus aureus* (*S. aureus*) or vancomycin-resistant *Enterococcus faecium* (*E. faecium*). Such strains, commonly referred to as „nightmare bacteria” with highly elevated resistance to last-resort antibiotics, have been reported all around the world in 2017. While silver, copper, zinc oxide or titanium dioxide have been used as surfaces or introduced as nanoparticles into a broad range of substrates to serve as antimicrobial agents and eradicate a wide range of pathogens, they all suffer from eventual reservoir depletion, and they tend to be pathogen- or condition-specific. Moreover, if not covalently bound or tightly embedded, these nanoparticles can leach into the environment and introduce additional health concerns. In this study, we discuss a photodynamic polymer composed of an olefinic thermoplastic elastomer modified with zinc tetra(4-N-methylpyridyl)porphine (ZnTMPyP4+), a photoactive antimicrobial, and demonstrate that this combination is remarkably effective at inactivating 5 bacterial strains, including *S. aureus* and *Escheria coli* (*E. coli*) often associated with food poisoning, and 3 different viruses, including Human adenovirus-5 and influenza type A, upon exposure to non-coherent light at an intensity of 65-80 mW/cm<sup>2</sup> for 60 min. By achieving antibacterial and antiviral efficacies of at least 99.89% and 99.95%, respectively, this methodology based on the light-induced creation of singlet oxygen constitutes a non-specific and highly efficient route by which to eliminate harmful pathogens via simple exposure to visible light and oxygen.

VISITING  
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CNBCh Research Group:  
**Wetland Ecology Research Group**  
headed by Prof. Wiktor Kotowski

## Dr. Hanna Silvennoinen

**University:** [Norwegian Institute for Bioeconomy Research](#)

**Country:** Norway

**Date of stay:**  
12–19 December 2018

### Activity at Home University:

Dr. Silvennoinen is a biogeochemist interested in carbon and nitrogen cycles and their regulation from micro- to ecosystem scale. She is currently working on multiple projects involving peatlands and organic soils.

### Activity at CNBCh UW:

Dr. Silvennoinen worked together with researchers at the Department of Plant Ecology and Environmental Conservation on data processing and interpretation of results from GHG concentration essay at Polish peatlands. On the 19<sup>th</sup> of December delivered a seminar: „Climate and peatlands – global challenge from arctic to tropic”.

### Prof. Wiktor Kotowski about cooperation

During her stay Dr. Hanna Silvennoinen worked on joined publication related to methane emissions from pristine fen mires with the members of Wetland Ecology Research Group. She also gave an open talk on the socio-economical aspects of carbon balance in boreal and tropical peatlands.

The visit resulted in preparation of the draft manuscript titled “No effect of the major ecohydrological gradient on methane production in temperate fens” and rising awareness among the CNBCh UW staff on the issue of the policy-related drivers of GHG emissions from peatlands. Future cooperation between Hanna Silvennoinen and the Wetland Ecology Research Group is expected. New project project applications are considered with the use of the funds of the Polish-Norwegian Research Programme.

# LECTURE

**VISITING  
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## Dr. Hanna Silvennoinen

Norwegian Institute for Bioeconomy Research

### Climate and peatlands – global challenge from arctic to tropic

**DATE:** 19 December 2018 | 13:00

**VENUE:** CNBCh UW, Hall B



CNBCh Research Group:  
**Laboratory of Biomodeling**  
headed by Prof. Sławomir Filipek

## Prof. Horst Vogel

### University:

[Ecole Polytechnique  
Fédérale de Lausanne  
\(EPFL\)](http://www.epfl.ch)

**Country:** Switzerland

### Date of stay:

25 February – 2 March  
2019

### Activity at Home University:

Professor of Biophysical Chemistry. Investigating cellular signaling using biophysical techniques including micro- and nanotechnologies, single-molecule spectroscopy and microscopy, structural biology (X-ray diffraction and cryo-electron microscopy) and molecular modeling.

His team concentrate on elucidating the structure and dynamics of membrane proteins such as G protein coupled receptors and channel proteins.

### Activity at CNBCh UW:

Lecturing on Cellular biochemical networks (CNBCh) and on Structure and Dynamics of Ligand-Gated Ion Channels (Tri-Bio-Chem programme). Consulting projects on Modelling Structure and Dynamics of Membrane Proteins in the Laboratory of Biomodelling headed by Prof. Sławomir Filipek.

### Prof. Sławomir Filipek about cooperation:

During his stay Prof. Horst Vogel delivered two lectures, one at CNBCh for general audience from Chemistry and Biology entitled "Imaging and manipulating cellular biochemical networks: from single-cells to single-molecules", and the second at Faculty of Chemistry for PhD students "Structure and dynamics of ligand-gated ion channels".

He also participated in seminar in Laboratory of Biomodeling providing valuable comments and visited Structural Biology Group for viewing the lab and discussions on protein structure determination problems. During all the stay Prof. Vogel made consultations on current projects performed in Laboratory of Biomodeling.

**Results of the visit:** The visit of Prof. Vogel was very helpful to discuss current progress in joint project which is going on, especially on involving more people in the research on G protein couple receptors which are very interesting from scientific point of view but also extremely importance as targets for drug design. Novel opportunities for collaborations were also discussed with emphasis on joint grant applications for EU Horizon 2020 programme".

# LECTURE

## Prof. Horst Vogel

Ecole Polytechnique Fédérale de Lausanne (EPFL)

**VISITING  
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### Imaging and manipulating cellular biochemical networks: From single-cells to single-molecules

**DATE:** Monday, 25 February 2019 | 12.00

**VENUE:** CNBCh UW, Hall B

### ABSTRACT:

Cellular signaling reactions are classically investigated by measuring optical or electrical properties in cell ensembles or individual cells. Miniaturized bioassays are of importance for example in basic research, clinical diagnostics and drug screening applications. Microfluidics and microarray technologies are currently used in this context but are limited to the analysis of nano- to picoliter volumes.

Here we show that cellular signaling cascades can be monitored in single, sub-micrometer-/attoliter-sized native vesicles derived from living cells. The vesicles comprise parts of a cell's plasma membrane and cytosol and represent the smallest autonomous containers performing cellular signaling reactions, thus functioning like minimized cells. We report on cellular signaling reactions mediated by ligand-gated ion channels and G-protein coupled receptors (GPCR) in native vesicles using combined single-molecule optical and electrophysiological techniques on a microfluidic chip. As a prototypical example, we measured in individual vesicles the different steps of GPCR signaling like ligand binding to receptors, subsequent G-protein activation and finally receptor deactivation via arrestin translocation.

Since many vesicles can be derived repetitively from a single cell over time and investigated as individuals, they are ideally suited for multiplexing single-cell analysis to study the heterogeneity between as well as within individual cells at different states of cell development and therapeutic treatment. This might be of interest for analyzing the diversity of rare primary cells, for example tumor or stem cells, with direct impact for personalized medical treatment.

# LECTURE

Prof. Horst Vogel

Ecole Polytechnique Fédérale de Lausanne (EPFL)

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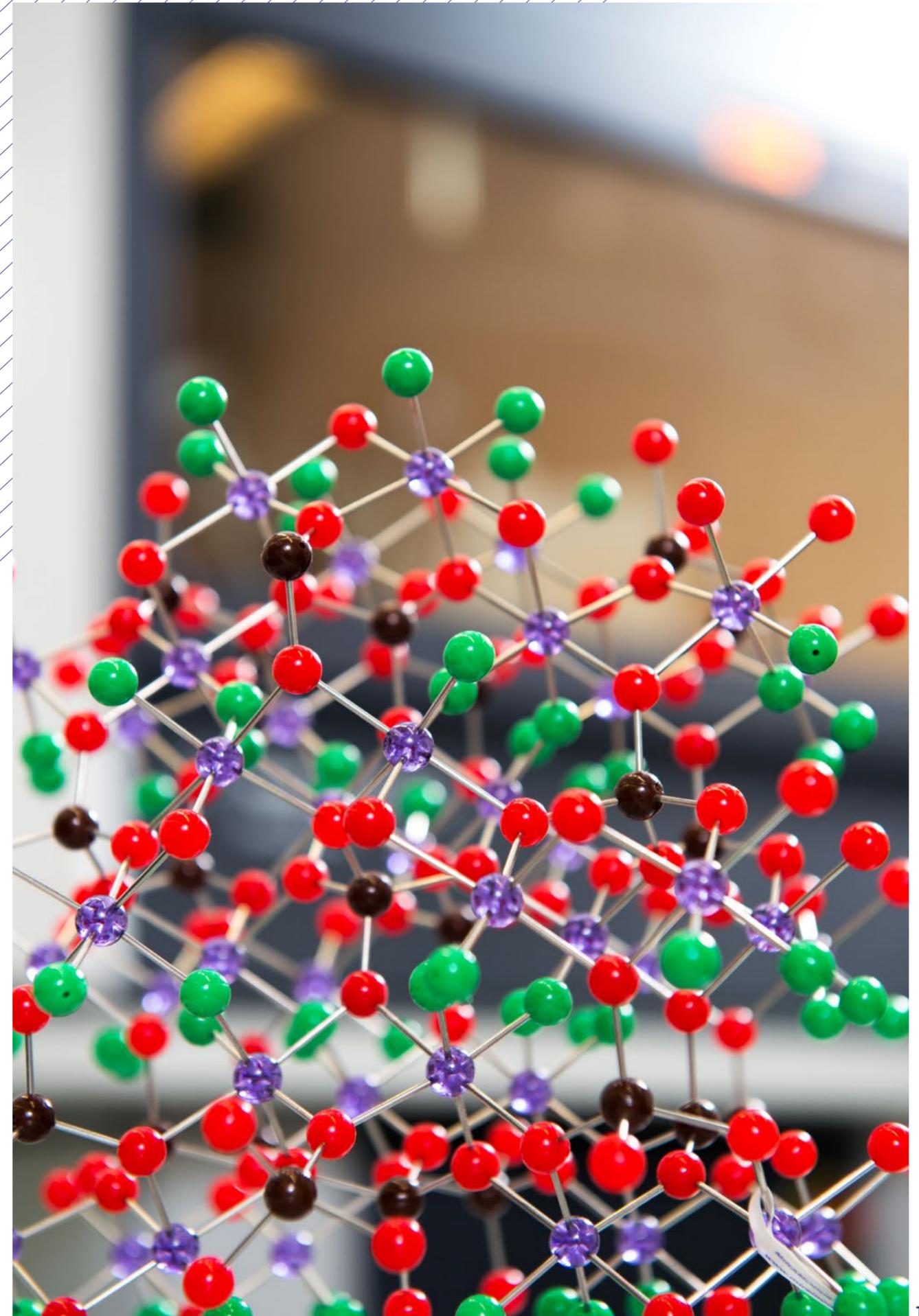
## Structure and dynamics of ligand-gated ion channels

**DATE:** Thursday, 28 February 2019 | 15.30

**VENUE:** CNBCh UW, Hall B

### ABSTRACT:

Neurotransmitter-gated ion channels of the Cys-loop receptor family mediate fast neurotransmission throughout the nervous system. The molecular processes of neurotransmitter binding, subsequent opening of the ion channel and ion permeation remain poorly understood. Here we review the progress in the field and present our own recent results of high-resolution X-ray crystallography, single particle imaging, and molecular modeling studies of a mammalian Cys-loop receptor, the mouse serotonin 5-HT<sub>3</sub> receptor. We revealed at atomic detail how neurotransmitter binding on the extracellular domain of the 5-HT<sub>3</sub> receptor induces sequential conformational transitions in the receptor opening a transmembrane ion channel: Agonist binding first induced distinct conformational fluctuations of particular side chains in the highly conserved ligand binding cage, followed by tilting-twisting movements of the extracellular domain which coupled to the transmembrane TM2 helices to open the hydrophobic gate and forming a continuous transmembrane water pathway. The structural transitions in the receptor's transmembrane part finally coupled to the intracellular region opening passages for ion release. The details of structural transitions of the 5-HT<sub>3</sub> receptor deliver important insights for understanding the activation mechanism of mammalian Cys-loop receptors.





CNBCh Research Group:  
**Structural Biology Group**  
headed by Dr. Maria Górna

## Prof. Ben Luisi

**University:** [University of Cambridge](#)

**Country:** United Kingdom, Cambridge

**Date of stay:**  
4–9 March 2019

### Activity at Home University:

Professor of structural biology, studies regulation of RNA metabolism and membrane transporters in bacteria. Elected as EMBO member and Faculty of 1000, multiple laureate of Wellcome Trust grants and holder of ERC Advanced Grant.

Prof. Luisi established a modern platform for CryoEM and CryoET at the Department of Biochemistry at the University of Cambridge. He was a PhD student of Max Perutz – Nobel laureate in chemistry in 1962 – in whose laboratory he worked on the structure of hemoglobin in LMB MRC in Cambridge together with Kiyoshi Nagai. He also studied protein-DNA interactions under the direction of Paul Sigler at the Yale University.

### Activity at CNBCh UW:

Professor, as a consultant of projects „Proteolysis-targeting strategies in bacterial systems for the development of antibiotics” and „Core facility for crystallographic and biophysical research to support the development of medicinal products”, joined the Structural Biology Group headed by Dr. Maria Górna and the Laboratory for Structural and Biochemical Research (LBSBio), headed by Prof. Krzysztof Woźniak.

### Dr. Maria Górna about cooperation

During his visit, Prof. Ben Luisi gave four different lectures:

- “Machinery of bacterial riboregulation”, as part of a mini-symposium with a guest from Poznań, Prof. Wojciech Rypniewski,
- a science and career talk for the “Do Science!” discussion club,
- “RNA-protein interactions in vivo and in vitro” – a lecture directed mainly at PhD students,
- “Structure and mechanism of multi-drug efflux assemblies”.

Prof. Luisi also took part in consultations and mentoring of team members for two projects:

- FNP First TEAM project “Proteolysis-targeting strategies in bacterial systems for the development of antibiotics?” – led by Maria Górna, Structural Biology Group
- FNP TEAM-TECH Core Facility project – Core facility for crystallographic and biophysical research to support the development of medicinal products – led by Krzysztof Woźniak, LBSBio

Ben Luisi also met with: representatives of the Polish Chapter of Marie Curie Alumni Association during a MCAA hangout, various researchers from the campus and the Departments of Biology, Chemistry and CeNT (for example:

Marcin Nowotny (IIMCB deputy director), Agnieszka Chacińska (CeNT director), Wiktor Koźmiński group (NMR group), Agata Krawczyk-Balska (molecular microbiology group).

**Results of the visit:** This visit reinforced the connections of the Structural Biology Group and LBSBio with Ben Luisi, who is the project partner in the First TEAM and TEAM-TECH Core Facility grants. It will make close collaboration easier, since our guest and team members had a chance to get to know each other better and to discuss research plans in detail. As an expert in CryoEM who established a modern CryoEM facility at his department, Ben Luisi gave valuable advice on how to arrange the local CryoEM infrastructure (at CeNT and IIMCB), the access to which is necessary for the future of structural biologists in our groups. His visit also helped to boost the local collaborations, for example between the Molecular Microbiology and Structural Biology Groups at CNBCh, which will work together on structural characterisation of sRNA-binding proteins from *Listeria monocytogenes*. The visit increased the visibility of our research in Warsaw scientific community and promoted science, researcher mobility and scientific careers.

# LECTURE

## Prof. Ben Luisi

University of Cambridge

### Machinery of bacterial riboregulation

**DATE:** Tuesday, 5 March 2019 | 11.00

**VENUE:** CNBCh UW, Hall B

#### ABSTRACT:

In many bacteria, ribonucleases play a central role in RNA processing and turnover as well as in RNA-mediated regulation. In *Escherichia coli* and other species, the enzyme RNase E serves as the scaffold of the RNA degradosome, which is a multi-protein assembly that is membrane-associated. We describe the components and organisation of the degradosome, and we present data that support a model for a highly dynamic assembly that can act cooperatively through allosteric conformational switching and clustering. A model will be described for how some sRNAs act in conjunction with the RNA chaperone Hfq to guide the machine to cleave targeted transcripts as part of intricate regulatory networks. Evidence for a recognition code for RNase E will be described, and a model presented for the stepwise process for interception, interrogation and handover of targeted substrate to the catalytic centers.

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CNBCh Research Group:  
**Laboratory of Surface Physicochemistry  
headed by Prof. Sławomir Sęk**

## Dr. Izabella Brand

**University:** [Carl von Ossietzky University of Oldenburg](#)

**Country:** Germany

**Date of stay:**  
1–15 April 2019

### Activity at Home University:

Researcher in physical Chemistry with focus on electrochemistry and bioelectrochemistry, Wittstock Group.

Research field: physical chemistry, electrochemistry, vibrational spectroscopy, surface science, adsorption of biomolecules at solid surfaces.

Research interest and experience: Modification of surfaces by functional, organized supramolecular films (in particular films of biomolecules), Electrochemistry of redox-active and redox-inactive molecules in thin organized films (e.g. amphiphilic organic molecules, amphiphilic metalosurfactants) and films of macromolecules (e.g. enzymes, polymers) adsorbed on electrode surfaces, Studies of the relationship between functions of molecular assemblies and their structure, Application of in situ structure analyzing techniques such as infrared reflection absorption spectroscopy to the electrochemical interface, Application of X-ray photoelectron spectroscopy to study surface composition of films adsorbed of solid surfaces.

### Activity at CNBCh UW:

- Lecturing on x-ray photoelectron spectroscopy (XPS),
- Discussion of results of a cooperation project on electrochemical and structural studies of model lipid bilayers obtained in the groups of Prof. Sęk and Dr. Brand,
- Preparation of a manuscript on electrochemical, spectroscopic and microscopic studies of potential driven changes in models of cell membranes of bacteria.

### Prof. Sławomir Sęk about cooperation

During the stay in Warsaw, Dr. Izabella Brand has delivered a series of lectures entitled "X-ray photoelectron spectroscopy for the analysis of surface". We have also analyzed and discussed the results obtained within our cooperation in the area of biomimetic lipid membranes. The results obtained so far might be a good starting point for the preparation of common scientific project.

Results of the visit: The measurable result of Dr. Brand's visit is the manuscript of the publication, which has recently been submitted to the "Bioelectrochemistry" journal. In the nearest future, we are planning to continue our cooperation, especially in the field of spectroelectrochemical studies of lipid membranes and their interactions with compounds of biological importance (e.g. antibiotics).

# LECTURE

## Dr. Izabella Brand

Carl von Ossietzky University von Oldenburg

### X-ray photoelectron spectroscopy for the analysis of surfaces

**DATE:** 2,3,4 April 2019 | 9:30

**VENUE:** CNBCh UW, Hall B

#### ABSTRACT:

The proposed lectures serve as an introduction to the X-ray photoelectron spectroscopy (XPS) and presentation of XPS as a superb analytical tool for chemical analysis of surfaces. First, phenomena occurring after bombardment of a solid surface with X-rays will be discussed. The measurement of the kinetic energy of an emitted electron allows the determination of the binding energy of an electron on a particular orbital of a particular element. The impact of the initial (prior to photoelectron emission) and final (after photoelectron emission) states on the binding energy will be discussed. It will be supported by examples from the literature. Characteristic features appearing in the XP spectra will be presented. XPS provides qualitative and quantitative information about an analyzed surface. The background of the quantitative and qualitative analysis of homo- and heterogeneous samples will be presented. The analysis of conductive samples in XPS is well documented in the literature. When a non-conductive sample is analyzed, some adjustment of experimental conditions is required. Modification of a conductive surface by molecular non-conductive films or corrosion of metallic surfaces changes electric properties of solid samples. Examples of studies of the composition and structure of self-assembled monolayers will be presented. The impact of the development of corrosive layer on a metallic surface will be presented.

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**Konrad Zawadzki**  
**Biological and Chemical Research Centre**  
**University of Warsaw**

## Prof. James Hoopes

**University:** Babson  
College, USA

**Country:** USA

**Date of stay:**  
1–15 April 2019

### Activity at Home University:

Murata Professor of Ethics in Business<sup>®</sup> at Babson College. His latest book is *Corporate Dreams: Big Business in American Democracy from the Great Depression to the Great Recession*. The author of half a dozen other books on American history, Hoopes has received grants from the Guggenheim Foundation, the Alfred P. Sloan Foundation, the National Endowment for the Humanities, and other funding agencies. His paper, „Managing a Riot,” won the Paul Hersey Award for the best paper on leadership at the 2000 meeting of the Academy of Management. He has taught in both Europe and Asia.

### Konrad Zawadzki about cooperation

Prof. James Hoopes is recognized as one of the top 5 business historians in the world. Currently, he is developing the concept of Moderate Ant-Corporatism looking for ways of the effective management without destroying such values as freedom of thought, equality and democratic ways of leading teams. These issues are also very important for the functioning of research teams in the competitive environment.

Prof. Hoopes during his visit - through lectures, workshops and seminars - share with participants the sensitivity to the danger of over-commercialization of research, and at the same time showed and discussed the effective use of non-corporative management traditions by research teams, both academic and those operating in the corporate environment. He proposed so called Moral Leadership, based on Character and Virtue as an effective and very human at the same time means of leading research groups in the competitive environment.

The main effect of the visit of Prof. Hoopes was an exchange of organizational experiences between Polish scientists, doctoral students and organizers of science and an experienced observer and critic of the contemporary world of organizations from the USA. The concept of Moral Leadership based on the Character and Virtues and its practical implications have been presented and discussed in the environment of strict science researchers for the first time in the world. Therefore, Polish researchers became the co-creators of one of the innovative management methods and its application to research teams. It resulted in further contact of the participants of the meetings with Prof. Hoopes, by Internet and in the interdisciplinary seminar in Poland, regularly discussing the Prof. Hoopes's proposals. One of the participants of the meeting with Prof. Hoopes is currently applying for a Fulbright Scholarship to work under Hoopes at Babson College. Steps to organize the next visits of Prof. Hoopes to Poland were also taken.

## LECTURE

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## Prof. James Hoopes

Babson College, USA

**How to use virtues oriented management, which is based on Buddhist traditions to improve researchers' teams leaders activity who try to commercialize the results of their studies? What is important to avoid from corporation world?**

**DATE:** Thursday, 3 April 2019 | 10.00

**VENUE:** CNBCh UW, seminar room 0.36



CNBCh Research Group:  
**Catalysis and Surface Science  
headed by Prof. Adam Lewera**

## Prof. Paul Bagus

**University:** [University of North Texas](#)

**Country:** USA

**Date of stay:**  
25 May – 10 June 2019

### Activity at Home University:

The principle scientific interest of Prof. Paul Bagus is to develop and apply theory and computation for the interpretation of core-level spectroscopies including XPS, XAS, and XMCD. These spectroscopies are routinely used non-destructive probes of material composition and properties. The aid of theory is needed for proper interpretation of these spectroscopies in terms of materials properties. Bagus' work on chemisorption has involved the use of cluster models to represent the surface electronic structure and, in particular, to describe the chemical interaction of adsorbed atoms and molecules with the surface. A special advantage of the cluster model is that it naturally allows chemical concepts to be used to interpret surface chemical bonding and surface reaction processes. His work related to surface electronic structure has addressed how this structure leads to observable properties. These have included work function changes, surface and nano-particle core-level binding energy shifts, and the nature of the chemisorption bond between adsorbates and substrates. For this latter research, he and his collaborators have developed a theoretical methodology that has allowed them to decompose different contributions to the chemisorption bond. For example, the application of his work to comparisons of the metal carbonyl bond has allowed direct understanding of the chemical reasons that, while p back-donation dominates for 3d transition metals, p back-donation and s donation are of comparable importance for heavier, 5d, transition metals. Understanding of adsorption processes allows for better understanding of heterogeneous activity of surfaces.

Research field: Theoretical chemistry, quantum mechanics, adsorption, X-ray Adsorption Spectroscopy, X-ray Photoemission Spectroscopy.

Research interest and experience: Professor Bagus carried out research on electronic structure of molecular and condensed systems, particularly on core-level spectroscopies. His research has been funded by many grants. Professor Bagus has over 350 publications, almost all relating to the electronic structure of matter. He is internationally recognized as a scientist and a member of national and international committees and societies.

### Activity at CNBCh UW:

Project consultation: XPS and NAP-XPS study of adsorption phenomena

### Prof. Adam Lewera about cooperation:

Prof. Paul Bagus had three lectures on adsorption and interpretation of photoelectron spectra. Additionally he was interpreting the data already collected by my group, as well as by other scientists.

**Results of the visit:** As a result we have gained the knowledge to interpret the subtle changes in photoelectron spectra due to adsorption. Additionally the results of multiplets on the spectra was presented. We plan further activity in cooperation with Prof. Bagus, such as joint research and joint papers.

# LECTURE

## Prof. Paul Bagus

University of North Texas, USA

**VISITING  
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### Theoretical Analysis and Understanding of Chemisorption

**DATE:** Tuesday, 28 May 2019 | 9.30

**VENUE:** CNBCh, seminar room 0.37

#### ABSTRACT:

The objective of this presentation is to show how chemisorption bonds can be analysed to identify the chemical and physical mechanisms responsible for the interaction and to show the consequences of the interaction for observed properties. An important result of this understanding is that it makes possible the correct interpretation of the relationship of observed properties to the nature of the surface chemical bond. The authors and their colleagues have pioneered in the development and application of theoretical methods that make it possible to identify the character of chemical interactions in terms of the concepts of molecular orbital theory. These methods will be applied to describe the bonding of common probe molecules, CO, CN, and NO, to different surfaces, including metals and insulators where the focus will be on the chemical content of the analysis rather than on the computational methods. The analysis will include interpretation of vibrational and photoemission spectroscopies and it will be shown how these spectra reflect the adsorbate-substrate interaction.

# LECTURE

Prof. Paul Bagus

University of North Texas, USA

VISITING  
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## Extracting Chemistry From the Analysis of Core-Level Spectra

**DATE:** Thursday, 30 May 2019 | 11.00

**VENUE:** CNBCh, seminar room 0.38

### ABSTRACT:

X-Ray Photo-electron Spectroscopy, XPS, is widely used to obtain information about both the composition and the chemical bonding of materials. The interpretation of the XPS in terms of chemical interactions is very commonly focussed on the shifts of core-level binding energies, BEs, to infer the chemical state of the material. In particular, a shift to higher BE is taken as indicating that the ionized atom is more positively charged, and the reverse is taken for shifts to lower BEs. However, there are other reasons for shifts in BEs besides charging; these include changes in hybridization and changes in bond distance. Furthermore, there are other features of the XPS besides BE shifts from which chemical properties of the material can be inferred. These include the number, width, and relative intensity of the main and satellite peaks of the often complex XPS spectra. The physical and chemical origins of these features allow them to be related, especially with guidance from theory, to the electronic structure of the material. An important mechanism is the angular momentum coupling of the open shell electrons which often leads to unresolved features and broad observed peaks.

# LECTURE

Prof. Paul Bagus

University of North Texas, USA

VISITING  
PROFESSOR  
PROGRAMME

## Multiplets: A Tutorial

**DATE:** Monday, 3 June 2019 | 11.00

**VENUE:** CNBCh, seminar room 0.38

### ABSTRACT:

A knowledge of multiplets is essential to understanding and interpreting all electronic spectra. This is true for both core and valence level spectroscopies. Multiplets have their origin in the angular momentum coupling of open shell electrons. They are the basis of selection rules and provide important information about the complexity of spectra including energy separations and relative intensities. A difficulty is that the fundamental theory of angular momentum coupling is based on a complex mathematical formalism. The objective of this tutorial is to show that there are simple rules that provide important information about the properties of multiplets and provide guidance for how the multiplet structure will be reflected in the electronic spectra.



CNBCh Research Group:  
**Environmentally Sensitive Polymer  
Materials and Composites  
headed by Dr. Marcin Karbarz**

## Dr. Jerzy Krzystek

**University:** National High  
Magnetic Field Laboratory

Florida State University,

**Country:** USA

**Date of stay:**  
10–15 June, 2019

**Activity at Home University:**

Research Faculty III at the MagLab  
(equivalent to Full Research Professor at FSU)

Research field:

Electron Spin/Paramagnetic Resonance at (very) high frequencies and magnetic fields (HFESR/EPR); Far-Infrared Magnetic Spectroscopy (FIRMS).

Research interest and experience:

Coordination chemistry of transition metals from the perspective of (a) catalytic activity, (b) bioinorganic chemistry and (c) single-molecule magnetic properties.

**Activity at CNBCh UW:**

Lecturing on applications of high magnetic fields in general, with particular emphasis on Dr. Krzystek's expertise in magnetic resonance as applied to materials science. Delivering a seminar presenting own research in the same area.

**Dr. Marcin Karbarz about cooperation:**

Activity during stay:

Dr. Krzystek gave series of lectures and seminars. In the lectures have participated the Scientist from CNBCh, Faculty of Chemistry, CeNT and Medical University of Warsaw.

Results of the visit:

A few Scientists working at CNBCh and Faculty of Chemistry declared their willingness to perform their research using instrumentation at the National High Magnetic Field Laboratory. Dr. Krzystek explained how it will be possible to apply for magnet time at the National High Magnetic Field Laboratory in the frame of user program.

# LECTURE

## dr. Jerzy Krzystek

National High Magnetic Field Laboratory (MagLab)  
Florida State University

**DATE:** 11-13 June 2019 | 10.00

**VENUE:** CNBCh, seminar room room 0.37

### Non-resonant high-field methods

**ABSTRACT:** Non-resonant high-field research generally strives to achieve highest possible magnetic field without much concern for its quality. I will start with presenting technologies applied to construct magnets generating increasingly higher fields, currently reaching thousands of teslas, although more routinely applied at the level of 100 teslas. I will then cover some applications of those fields in the area of materials science, which is mainly materials/solid state physics.

### Advanced magnetic resonance in high fields

**ABSTRACT:** In contrast to non-resonant methods, magnetic resonance generally requires high homogeneity and therefore necessitates different magnet technologies, mainly based on superconducting materials. I will cover the prevailing trends in superconducting magnet design which recently achieved 32 teslas, and prospectively may attain 40-tesla level. After covering the advantages of high fields in NMR, MRI and ICR (ion cyclotron resonance), I will turn to my own area of expertise, HFEP (high-frequency and -field electron paramagnetic resonance). Advanced HFEP techniques will be presented and discussed, including applications in materials science, particularly materials chemistry.

### High-frequency and -field Electron Paramagnetic Resonance (HFEP) applied to certain perovskites

**ABSTRACT:** A perovskite-type material of general formula:  $\text{YIn}_{1-x}\text{Mn}_x\text{O}_3$  with  $0.02 < x < 0.2$  displays very unusual optical properties in that for modest Mn(III) ion content it displays intense blue color, very unusual for manganese compounds. This property has already been applied in creating versatile blue pigments. In my presentation I will cover the history of the quest for a perfect blue dye and/or pigment dating back to ancient Egypt and China. More recently, we have investigated the correlations between the optical (i.e. electronic) properties with magnetic ones via HFEP. In particular, spin Hamiltonian parameters of the ground quintet ( $S=2$ ) spin state of manganese(III) can be linked to the electronic structure of that ion on several levels of theory, starting with a simple ligand-field approach more typically applied in coordination chemistry.

**VISITING  
PROFESSOR  
PROGRAMME**



CNBCh Research Group:  
**Structural and Biochemical Research  
Laboratory headed by  
Prof. Krzysztof Woźniak**

## Prof. Delia Haynes

**University:** [Stellenbosch University](#)

**Country:** South Africa

**Date of stay:**  
7–14 July 2019

### Activity at Home University:

Prof Haynes is an Associate Professor in the Department of Chemistry & Polymer Science at Stellenbosch University. She lectures inorganic chemistry and is part of a group of researchers who work in supramolecular chemistry.

**Research field:** Research in the Haynes group is in the general area of crystal engineering, or solid-state supramolecular chemistry. We work on organic multi-component crystals (salts and co-crystals), and aim to understand and use intermolecular interactions to design molecular materials with interesting and useful physical properties. In particular we study porous organic salts, and also investigate organic radicals as building blocks for molecule-based magnetic and conducting solids. Research focuses on the interplay between solid-state structure and function, as well as the effect crystallisation method has on the structure and properties of the resulting material.

**Research interests and experience:** Prof Haynes' research focuses on crystal engineering with multi-component crystals. She has experience both with thi-azyl radicals as building blocks for molecular materials, and with organic salts and co-crystals. Delia was a Fulbright Scholar at the University of California, Berkeley in 2010, a visiting professor at the University of Lorraine in 2013, and was the 2015 recipient of the Jan Boeyens medal. She is a member of the Executive Committee of the European Crystallographic Association, and the chair of the Steering Committee for the African Crystallographic Association.

### Prof. Krzysztof Woźniak about cooperation:

During her visit, professor gave two different lectures: (1) "Towards functional materials from multi-component crystals" (2 30pm, Tue, 9/07/2019, room 0.38, CNBCh), (2) "Unusual methods of crystallisation: mechanochemistry and sublimation" (ca. 1 hr later than the first lecture). She also took part in consultations and mentoring of team members for two projects: (i) FNP TEAM-TECH "Core Facility project - Core facility for crystallographic and biophysical research to support the development of medicinal products" - led by Prof. Krzysztof Woźniak, and (ii) NCN OPUS "Advancing quantum crystallography for better insight into structure and properties of crystals" - also led by Prof. Krzysztof Woźniak. Additionally, we discuss prospects of further cooperation between her group from Stellenbosch University and my group from CNBCh UW.

This visit reinforced the connections of the Laboratory for Structural and Biochemical Research with Prof. Delia Haynes and her group from Stellenbosch (SA) who is a rising star of international science. Delia was selected to represent African science at the panel of leading young scientists at the very special meeting opening of the year of Crystallography. Delia's visit will make our close collaboration easier, since our guest and team members had a chance to meet and discuss different scientific opportunities and to see experimental possibilities at our group and Institute. Delia's visit also helped us to boost our joint collaboration as we agreed on joint application to Advanced Photon Source (APS, Chicago, USA) entitled: "Understanding of the nature of the interactions between  $\pi$ -radical dimers in 1,2,3,5-dithiadiazolyl radical crystals - formation of new covalent bonds under pressure". Unfortunately, the pandemic of COVID slowed down our joint activities.

# LECTURE

## Prof. Delia Haynes

University of Stellenbosch

### Towards functional materials from multi-component crystals

**DATE:** Tuesday, 9 July 2019 | 15:30

**VENUE:** CNBCh, seminar room 0.38

#### ABSTRACT:

Multi-component crystals, which include both salts and co-crystals, offer several advantages in the development of organic materials. Properties such as flexibility and solubility, as well as the possibility of including desirable physical properties in a material without altering key molecular properties, make multi-component crystals attractive targets. This lecture will describe efforts in our group to develop multi-component crystalline materials with interesting physical properties.

Co-crystallisation has been investigated as a means of overcoming dimerization in 1,2,3,5-dithiadiazolyl radicals (hereafter DTDAs). DTDAs are of considerable interest due to their potential as building blocks for organic magnetic or conducting materials, but they frequently dimerise in the solid state, rendering them diamagnetic. Co-crystallisation initially seemed a promising route to overcoming dimerisation in DTDA radicals, however this has proven to be more challenging than expected. A computational investigation, as well as experimental charge density studies, have been carried out on some DTDAs and DTDA co-crystals in order to better understand the dimerisation interaction. Insight gained from these studies will be discussed.

Porous organic salts offer several advantages over metal-organic frameworks and covalent organic frameworks; for example these materials can be dissolved and re-assembled from solution. We have investigated the use of the pamoate ion in the design of porous organic salts. The interesting properties of several salts, including selectivity and guest exchange, will be presented. Recent results involving a series of zwitterionic building blocks will also be discussed.

**VISITING  
PROFESSOR  
PROGRAMME**

# LECTURE

Prof. Delia Haynes

University of Stellenbosch

VISITING  
PROFESSOR  
PROGRAMME

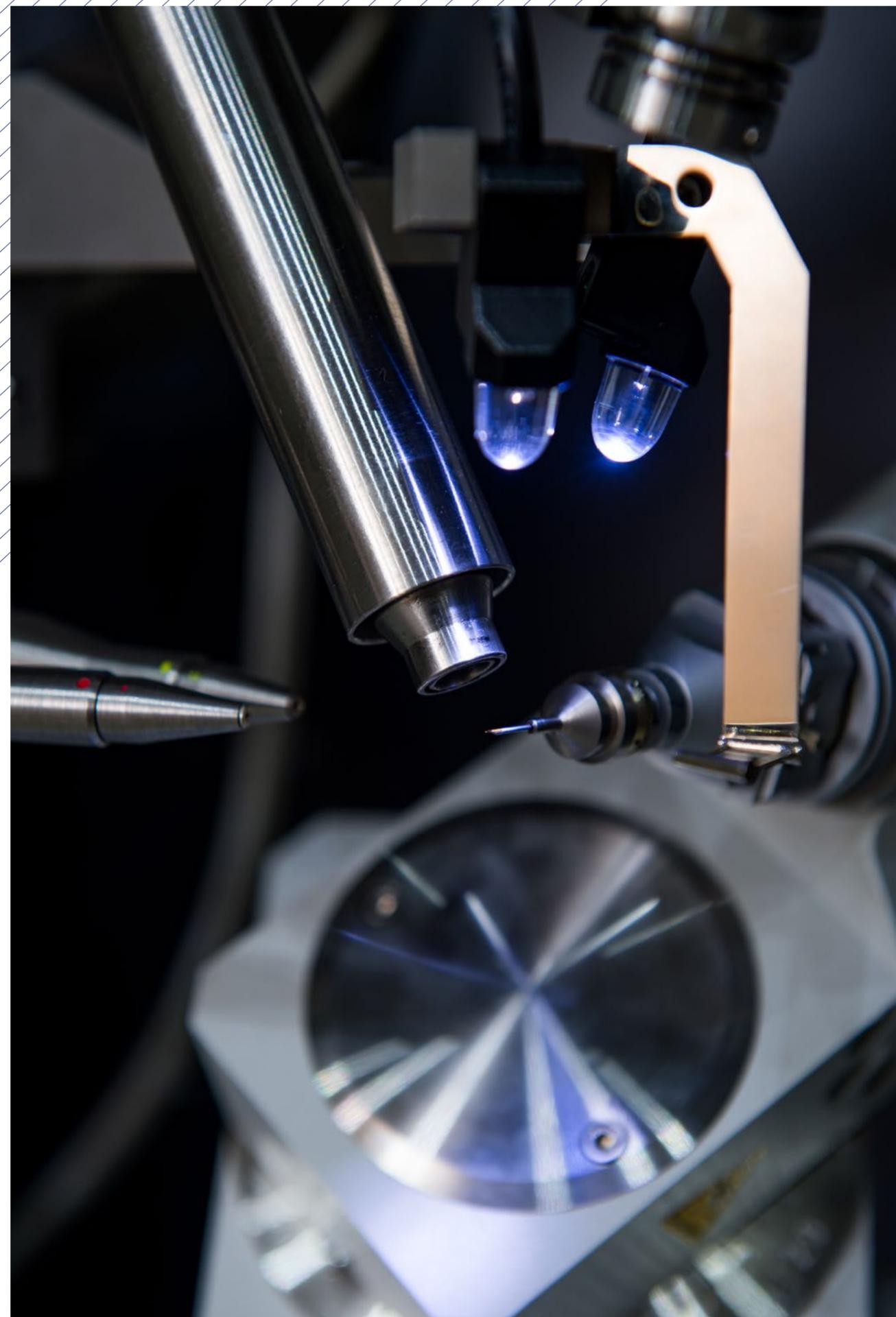
## Unusual methods of crystallisation: mechanochemistry and sublimation

**DATE:** Tuesday, 9 July 2019 | 14.30

**VENUE:** CNBCh, seminar room 0.38

### ABSTRACT:

Conventionally, crystals are grown using solvent-based methods such as slow evaporation or diffusion of an anti-solvent. There are, however, a number of lesser-known crystallisation methods. These can sometimes yield materials that are impossible to obtain in any other way. In this lecture, we will discuss the use of both mechanochemistry and sublimation to produce crystalline materials. Advantages and disadvantages of each method will be discussed, as well as practical considerations when using these techniques. An overview of some relevant literature and recent results in this area will also be presented.





CNBCh Research Group:  
**Analytical Expert Centre**  
 headed by Prof. Ewa Bulska

## Dr. Rafal Gutaker

**University:** [New York University](#)

**Country:** USA

**Date of stay:**  
 25 July – 3 August 2019

### Activity at Home University:

I am a Postdoctoral Associate at the Center for Genomics and Systems Biology, New York University. I lead research projects on comparative genomics of crop plants and method development for plant ancient DNA.

**Research field:** Ancient DNA revolutionized the field of evolutionary biology for humans and ignited that revolution for other model and non-model organism. Plant ancient DNA can help us better understand the origins of crops, their dispersal and evolution in different environmental conditions. This is very important because our food security relies heavily on the diversity of our crops and their ability to evolve in response to changing climate.

**Research interests and experience:** Throughout my academic career I was driven by passion for history, evolution and plant biology. I completed my PhD at the University of Warwick working on ancient genomics. Since 2014, I have worked as a postdoctoral fellow at the Max Planck Institute for Developmental Biology developing laboratory protocols and computational approaches to compare ancient and modern genomes of plants. In 2017, I became a postdoctoral associate at New York University to lead research on the effects of the environment on crop evolution.

### Activity at CNBCh UW:

Presented a lecture on the developments in ancient DNA techniques and their utility in studying crop genomes. Also was a consultant of the research groups at CNBCh and CeNT about the operations of new generation sequencing core facilities.

### Professor Ewa Bulska about cooperation:

During his reserach visit Dr. Gutaker presented his research on the seminar organised by ACE reseach group. The information was spread withing all institution on Ochota Campus. The seminar entitled "New generation sequencing and ancient DNA in the service of plant evolutionary genomics" (August 1, 2019). During the visit several face to face meetings were organised and a numebr of scientists had an oportunity to discussed their research in the field of NGS.

Results of the visit: The main advantageous of the visit of Dr. Gutaker, expressed by young scientist, was the possibility to discussed not only the direct issue of advantages of including NGC results in various reserach projects. Extremally important was the possibility to discus the advantageous and difficulties of performin scientific carriers abroad. Dr. Gutaker was able to share his experience and give several advise for young scientists on how to plan individual carrier.

# LECTURE

## Dr. Rafał Gutaker

Center for Genomics and System Biology  
 New York University

**VISITING  
 PROFESSOR  
 PROGRAMME**

### New generation sequencing and ancient DNA in the service of plant evolutionary genomics

**DATE:** Thursday, 1 August 2019 | 11.00

**VENUE:** CNBCh, seminar room 0.38

### ABSTRACT:

The advances in sequencing technologies and improved methods for retrieval of ancient DNA made it possible to sequence whole genomes of long-dead organisms. While the most impressive discoveries thus far were made for humans, there are growing possibilities and growing demand to analyze historical and ancient genomes of plants. All the methods applied to human aDNA can be used directly, or with small modifications, to analyze plant aDNA. Highlighted by work on potato, maize and rice that I have lead, I would like to exemplify how whole genome data of historical and ancient specimens helped in understanding the processes of crop dispersal and adaptation. Historical genomics allowed tracing the complex origin and adaptation history of European potato. Our study helped us gain a deeper understanding of the potato introduction to Europe, where it adapted to very different environment compared to the place of its origin, South America. Moving back in time, our investigation of maize ancient genomes allowed us to reconstruct its North American dispersal in the context of shift from tropical to temperate climate. Finally, our reconstruction of rice dispersal based on the contemporary diversity of genomes revealed strong association with paleoenvironmental and archaeological transitions in Asia. The lack of aDNA data for rice present a major hurdle in our understanding of the key aspects of rice evolution.



CNBCh Research Group:  
**Analytical Expert Centre  
headed by Prof. Ewa Bulska**

## Dr. Lu Yang

**University:** [National Research Council Canada](#)

**Country:** Kanada

**Date of stay:**  
2–7 September 2019

### Activity at Home University:

Dr. Lu Yang is a senior research officer at National Research Council of Canada (NRC, Ottawa, Canada), leading research in applications of inductively coupled plasma mass spectrometry (ICP-MS) and multicollector (MC-ICP-MS). A member of the IUPAC Subcommittee on Stable Isotope Reference Material Assessment under the Inorganic Division, and the Commission on Isotopic Abundances and Atomic Weights. She is a NRC's representative at the Isotope Ratio Analysis Working Group of CCQM (Consultative Committee for Amount of Substance) of the BIPM (International Bureau of Weights and Measures). She is an Editorial Board member of JAAS and Spectroscopy.

**Research field:** Her research focuses on the development of the most accurate and precise methodologies for the determination, speciation and isotopic analysis of trace elements using ICP-MS and MC-ICP-MS. The isotopic measurements for mercury, germanium, indium, iridium, osmium, hafnium and lead from her lab have been adopted by IUPAC as the best available isotopic composition measurements in the 2013, 2017 and 2019, and the standard atomic weights of mercury, germanium, iridium and hafnium are based on her lab results. She has published over 125 peer reviewed publications and a book chapter, with H-index of 33.

### Activity at CNBCh UW:

Dr Lu Yang presented one lecture during her stay: Applications of MC-ICPMS for high accuracy and precision isotope ratio measurements at NRC

### Professor Ewa Bulska about cooperation:

During one week visit Dr. Lu Yang presented invited lecture in the frame of analytical chemistry section in the frame of the national congress of chemistry "62. Zjazd Naukowy PTChem". Lecture title "Applications of MC-ICPMS for high accuracy and precision Isotope Ratio Measurements at NRC" (September 3, 2019). Then, Dr Lu presented the lecture on the scientific seminar organized by CNBCh UW. The seminar was organized by ACE research group. Title of presentation "Principle and use of MC-ICPMS for high accuracy and precision Isotope Ratio Measurements for selected application" Moreover several meetings were organized both face to face discussion as well as common work at the laboratory towards implementation of Optimised Regression Model

**Results of the visit:** As a main result of the research visit we consider the common publication in highly ranking journal Anal Chem was recently accepted for publication. Karasinski, Jakub; Tupys, Andriy; Yang, Lu; Mester, Zoltan; Halicz, Ludwik; Bulska, Ewa. "A Novel Approach for the Accurate Determination of Se Isotope Ratio by Multicollector ICP-MS" Journal: Analytical Chemistry; Manuscript ID: ac-2020-03768k.R2".

# LECTURE

## Dr. Lu Yang

National Research Council Canada

### Applications of MC-ICPMS for high accuracy and precision isotope ratio measurements at NRC

**DATE:** 5 September 2019 | 10.00

**VENUE:** CNBCh, seminar room 0.37

#### ABSTRACT:

High precision and accuracy isotope ratio measurements have played central role in many disciplines from studies of early solar system formation and age dating in geoscience to studies in medical science, nuclear and forensic sciences, and environmental science etc.1-2 Currently multi-collector inductively coupled plasma mass spectrometry (MC-ICPMS) is a powerful tool for such measurements, providing the instrumental isotopic fractionation/mass bias is properly dealt with, which is not trivial.3 In addition to commonly believed mass-dependent fractionation (MDF), mass-independent fractionation (MIF) has been reported in MC-ICPMS itself for many elements including Nd4-7, Ce5, W8, Sr5, 9, Ge10, Pb10, Hg10, Si11, Ba12, Os13 and Hf14-15, which has a huge impact on the choice of mass bias correction models. Most applications of isotope ratio measurements rely on SI traceable isotopic standards to calibrate the instruments. Unfortunately, many elements still lacks SI traceable isotopic standard and measurements, thus, researchers are forced to use different commercial standard solutions as delta zero to report isotope ratios in a delta notation ( $\delta = (R_{\text{sample}}/R_{\text{standard}} - 1) \times 1000$ ), making isotope ratios measured world-wide incomparable. In the last decade, many international Metrology Institutes including NRC have made significant efforts in the development and the certification of isotopic standards.

Among many mass bias correction models, without rely on isotopic standard of the analyte, two state-of-the-art mass bias correction models2 are capable of correcting both MDF and MIF. One is the primary method, so called full gravimetric isotope mixture (FGIM) model, which is based on use of all near-pure isotopes of an element (e.g., all four isotopes of 204Pb, 206Pb 207Pb and 208Pb) with known chemical purities to prepare gravimetric mixtures, without rely on any existing isotopic standards and prior knowledge of isotopic composition of the near-pure isotopes. The second model is the optimized regression model and it presents as an alternative/secondary method for absolute isotope ratio measurements. This method allows calibrating isotope ratios of an element using a known isotope ratio of another element without assuming that the two elements must necessarily display identical mass bias (they do not). Recent research results from our group will be presented and discussed in details in this lecture.

**VISITING  
PROFESSOR  
PROGRAMME**



CNBCh Research Group:  
**New Materials Electrochemistry  
headed by Prof. Rafał Jurczakowski**

## Prof. Andrzej Lasia

**University:** [Université de Sherbrooke](#)

**Country:** Canada

**Date of stay:**  
2–13 September 2019

### Activity at Home University:

Professeur titulaire until 2012 and now Retired professor. Scientific collaborations with colleagues in the Department and outside.

### Research field:

Fundamental electrochemistry and electrocatalysis, theory and applications of the electrochemical impedance spectroscopy, porous electrodes, hydrogen adsorption, absorption, and evolution.

### Research interests and experience:

Development and characterization of new materials for hydrogen evolution, hydrogen absorption in palladium and its alloys and AB<sub>5</sub> materials, kinetics of hydrogen underpotential deposition on noble metals.

### Activity at CNBCh UW:

Lectures (30 h) on the electrochemical impedance spectroscopy and its applications.

### Prof. Jurczakowski about cooperation:

#### Activity during stay:

Prof. Andrzej Lasia held a 30-hour course "Electrochemical Impedance Spectroscopy and its applications". During the course, Prof. Andrzej Lasia presented a modern and complete review of the subject of electrochemical impedance spectroscopy. Prof. Andrzej Lasia presented mathematical development of the fundamental equations in impedance spectroscopy. The course was attended by young researchers, PhD students from University of Warsaw, Warsaw University of Technology and Polish Academy of Sciences. An important part of the course were practical computer exercises on simulation of impedances, Fourier transform data analysis, determination of impedance parameters, data modeling and Kramers-Kronig transformations. Professor Andrzej Lasia has provided also project consultations for researchers from University of Warsaw faculty of Chemistry, Warsaw University of Technology and Poznan University of Technology.

#### Results of the visit:

Prof. Andrzej Lasia provided also important and fruitful project consultations for researchers from University of Warsaw faculty of Chemistry, Warsaw University of Technology and Poznan University of Technology that were highly appreciated. Prof. Andrzej Lasia participated also in research projects held in group of Prof. Jurczakowski related to hydrogen absorption on platinum group metals and hydrogenation reactions, determination and modeling of kinetics of hydrogenation reactions and modeling of hydrogen adsorption isotherms on platinum metals. Young researchers and PhD students acquired deep understanding of the theory and applications of impedance spectroscopy.

# LECTURE

## Prof. Andrzej Lasia

Université de Sherbrooke, Sherbrooke

### Electrochemical Impedance Spectroscopy and its applications

**DATE:** 2–13 September 2019 | 9.00

**VENUE:** CNBCh UW, seminar room 0.37

#### ABSTRACT:

Electrochemical Impedance Spectroscopy (EIS) have seen tremendous increase in popularity in recent years. Initially applied to the determination of the double-layer capacitance and in ac polarography, they are now applied to the characterization of electrode processes and complex interfaces, batteries and fuel cells, corrosion, coatings and paints, supercapacitors, membranes, semiconductors, etc. EIS studies the system response to the application of a periodic small amplitude ac signal. Analysis of the system response contains information about the interface, its structure and reactions taking place there. EIS became very popular in the research and applied chemistry.

However, EIS is a very sensitive technique and it must be used with great care. Besides, it is often very poorly understood. This may be connected with the fact that existing reviews on EIS are very often difficult to understand by non-specialists and, frequently, they do not show the complete mathematical developments of equations connecting the impedance with the physico-chemical parameters. It should be stressed that EIS cannot give all the answers. It is a complementary technique and other methods must also be used to elucidate the interfacial processes.

The purpose of this lecture is to fill this gap by presenting a modern and relatively complete review of the subject of electrochemical impedance spectroscopy, containing mathematical development of the fundamental equations. The lecture includes computer exercises on simulation of impedances, Fourier transform data analysis, determination of impedance parameters, data modeling, and Kramers-Kronig transforms.

**VISITING  
PROFESSOR  
PROGRAMME**



CNBCh Research Group:  
**New Materials Electrochemistry  
headed by Prof. Rafał Jurczakowski**

## Prof. Tamas Pajkossy

**University:** [Hungarian Academy of Sciences](#)

**Country:** Hungary

**Date of stay:**  
2–13 September 2019

### Activity at Home University:

Areas of professional interest are related to electrochemistry as:

- connection of electrode kinetics and electrode geometry in general (1983-) and connection of electrochemistry and fractal geometry in particular (1983-1990)
- double layer properties of metal electrodes, with and without adsorption effects (1994-)
- perturbation methods and related instrumentation (1981-); dynamic electrochemical impedance spectroscopy (2015-) – and as a byproduct of these studies: development of various test instruments for the Hungarian lamp industry (1977-2005)

Teaching activities: various courses on electrochemical and physico-chemical instrumentation for chemical engineering students of TU Budapest

### Activity at CNBCh UW:

Preparation of electrochemical experiments – mostly of dynamic electrochemical impedance spectroscopy, DEIS – to study the electrochemical double layer on noble metals. Delivered a lecture on a novel method of data evaluation of DEIS.

## LECTURE

### Prof. Tamás Pajkossy

Hungarian Academy of Sciences

**VISITING  
PROFESSOR  
PROGRAMME**

### Analysis of voltammograms and impedance spectra of quasi-reversible redox system: transformation to program independent form

**DATE:** 4 September 2019 | 9.00

**VENUE:** CNBCh UW, seminar room 0.38

#### ABSTRACT:

A simple procedure is suggested by which cyclic voltammograms, CVs, pertinent to partially diffusion controlled charge transfer reactions can be analyzed. By this procedure, from a set of CVs taken at varied scan rates, two scan-rate independent, hysteresis-free functions can be calculated. One of them is the diffusion-free polarization curve,  $j_{inf}(E)$ , the other is the semiintegrated form of the reversible CV,  $M_{rev}(E)$ .

By analysing the electrochemical impedance spectra (EIS) of quasi-reversible redox systems, the two elements of the Faradaic impedance: charge transfer resistance and the coupled Warburg-coefficient can be obtained at a given potential. The same applies also to DEIS (dynamic EIS) measurements, when high frequency impedance spectra are measured while the potential is scanned to simultaneously accomplish cyclic voltammetry or other transient measurements. In case of DEIS both the charge transfer resistance and the Warburg coefficient depend on the applied potential program, e.g. on scan-rate. A theory is presented, yielding a transformation by which this dependence can be eliminated. The proposed procedure yields two, scan-rate independent, hysteresis-free functions, which are closely related to the EIS results, and also to the functions which are the transformed forms of the cyclic voltammograms (see the above plots).

In the lecture the mathematics of these ideas are presented illustrated with simulation results.



CNBCh Research Group:  
**Biochemistry, Ecology and Environmental  
Protection, Headed by Prof. Małgorzata  
Suska-Malawska**

## Prof. Svetlana Rogacheva

**University:** Saratov  
Medical University  
"REAVIZ"

Yuri Gagarin State  
Technical

University of Saratov,  
Russia

**Country:** Russia

**Date of stay:**  
7–22 October 2019

### Activity at Home University:

Research associate of Saratov Branch of All-Russian Institute of Genetics & Selection of Industrial Microorganisms (1988-1998); Associate Professor in Saratov Military Institute of Biological and Chemical Safety (1998-2009); Head of the Chair "Nature & Technosphere Safety" in Yuri Gagarin State Technical University of Saratov (2009–2018). Present workplace: Head of the Chair of Natural Sciences of Saratov Medical University "REAVIZ", Professor of the Chair "Nature & Technosphere Safety" of Yuri Gagarin State Technical University of Saratov, Russia.

Areas of professional interest are related to biochemistry, biophysics, ecological biotechnologies, as:

- Microbial enzymes, catalyzing the process of nitrile transformation into amide and acid; microbial biosensor systems for acrylamide and acrylonitrile determination in water (1988-2001).
- Nonspecific effect of physiologically active and toxic compounds in combination with electromagnetic radiation of low intensity on biological systems and their models (2001-2015).
- Solid-surface fluorescence of polycyclic aromatic hydrocarbons and heteroaromatic compounds for using in chemical sensors (2013-present).

Teaching activities: lectures and workshops for students of Yuri Gagarin State Technical University: "Fundamentals of biochemistry", "Fundamentals of microbiology and biotechnology", "Xenobiotics", "Biological indication and biological testing", "Chemistry and biology for engineers-ecologists", "Environmental protection and technologies of its rehabilitation", lectures and workshops for students of Saratov Medical University "REAVIZ" in "Bioorganic chemistry".

### Activity at CNBCh UW:

Preparation of luminescent experiments with some organic components of soils, especially using the method of solid surface fluorescence on the diacetate cellulose matrices. Delivering a lecture on biosensors and chemical sensors of toxic compounds.

### Prof. Małgorzata Suska-Malawska about cooperation:

During her stay Prof. Svetlana Rogacheva gave a lecture for researchers and a lecture for students from Environmental Management M.Sc. course. In addition, in Laboratory of Biogeochemistry and Environmental Protection scientific experiments were performed using the luminescence technique to detect PAH compounds.

**Results of the visit:** The results obtained during experiments will be elaborated and published in scientific journal. We plan to prepare a small pilot grant, too.

## LECTURE

### Prof. Svetlana Rogacheva

Saratov Medical University "REAVIZ",  
Yuri Gagarin State Technical University of Saratov, Russia

**VISITING  
PROFESSOR  
PROGRAMME**

### Biosensors and chemical sensors of toxic compounds

**DATE:** Monday, 14 October 2019 | 13:00

**VENUE:** CNBCh UW, Hall B

#### ABSTRACT:

One of the urgent tasks of chemical analysis is the fast, not requiring complex sample preparation, selective determination of low concentrations of toxic substances in natural environments, food, raw materials, biological fluids. The solution of such a complex problem is possible with the help of chemo- and biosensors. These are devices that selectively react to a defined substance due to a chemical reaction or physical process taking place on a sensitive (recognition) element of a chemical or biological nature, and convert the result of the reaction into an easily recorded signal using a transducer.

Modern sensors are a product of the integration of achievements in various fields of knowledge - chemistry, biology, physics, mathematics and microelectronics. The lecture summarizes information on sensitive elements and transducers used in chemo- and biosensors, analytical characteristics and application of sensor systems.

Particular attention is paid to electrochemical and optical sensors. The principles of their construction, chemical and biochemical reactions underlying the action of their sensitive elements are considered. Examples of using sensors of these classes for the determination of toxic compounds are given. The results of our own research of sensitive elements of the amperometric biosensor of acrylic acid derivatives and the fluorescent chemosensor of polycyclic aromatic hydrocarbons are discussed. The results of the study of Saratov scientists on the development of potentiometric, immunochemical sensors and "electronic nose" are presented.



CNBCh Research Group:  
**Laboratory of Physicochemistry  
of Materials headed by Prof. Robert  
Szoszkiewicz**

## Prof. Krzysztof Kuczera

**University:** University of Kansas

**Country:** USA

**Date of stay:**  
3-10 January 2020

**Activity at Home University:**

Professor in the Department of Chemistry and the Department of Molecular Biosciences.

**Research field:** Computational chemistry and biochemistry.

**Research interest and experience:** The research goal is to determine detailed microscopic effects of the environment on peptide structure, dynamics and interactions with proteins. Our studies employ molecular dynamics, replica-exchange and free energy simulations, as well as kinetic network modeling, to provide microscopic insights into influence of temperature, pH, viscosity and presence of co-solvents on peptide folding pathways. Our work involves extensive collaborations with experimental groups.

**Teaching activities:** Courses in general chemistry, physical chemistry, quantum chemistry, statistical mechanics and advanced biochemistry. I am especially interested in creating opportunities for students to experience molecular and data modeling, introducing active learning elements into the classroom and developing approaches for improving diversity and equity in science education.

**Activity at CNBCh UW:**

Visiting Professor presented a seminar and was developing a joint simulation-experimental project with Prof. Robert Szoszkiewicz.

### Prof. Robert Szoszkiewicz about cooperation:

- An invited lecture about peptide folding being simulated using novel molecular dynamics methods.
- Consultations with other CNBCh and UW Chemistry scientists regarding methods and force-fields used in MD simulations, and in particular discussion with the group of Dr. Agata Królikowska from UW Chemistry.
- Major consultations and work for the purpose of the NCN Harmonia 10 project led by Prof. R. Szoszkiewicz. This grant is about novel methods of detecting small structural changes within surface adsorbed peptide films.

**Results of the visit:** Apart of delivering a lecture and discussing with other UW scientists Prof. K. Kuczera has performed two 10-microsecond MD simulations of the alpha-helix-forming peptide Ac-(AAQAA)<sub>3</sub>-NH<sub>2</sub>, using the CHARMM36m protein force field with TIP3P

water model. All for the purpose of the collaboration with Prof. R. Szoszkiewicz within the NCN Harmonia 10 project. One simulation has started with a helical, the other one with an extended peptide conformation. The simulations show multiple folding and unfolding events. The peptide samples a large conformational space, which is similar in both trajectories. The relaxation times are in the 10-100 ns time range. These results are the basis for the understanding of the microscopic behavior of this system by itself and when crowded with other similar structures in the near neighborhood (as in the peptide film adsorbed on a smooth surface). Interpretation of these and upcoming results and their connection to the experimental studies under way at CNBCh within the group of Prof. Szoszkiewicz are subjects for future cooperation.

# LECTURE

## Prof. Krzysztof Kuczera

Department of Chemistry and Department of Molecular Bioscience  
University of Kansas

VISITING  
PROFESSOR  
PROGRAMME

### Multiple timescales of peptide folding from computer simulations

**DATE:** Thursday, 9 January | 11:00  
**VENUE:** CNBCh UW, room 0.38

**ABSTRACT:**

Long-term molecular dynamics simulations and a novel kinetic coarse-grained analysis were carried out to model the mechanism of formation of the helix-coil transition in a 21-residue peptide. A 12 microsecond molecular dynamics trajectory in explicit solvent yielded structural and dynamic properties in good agreement with available experimental data. Clustering and optimal dimensionality reduction were applied to produce low-dimensional coarse-grained models of the underlying kinetic network in terms of 2-5 metastable states. In accord with the generally accepted understanding of the multiple conformations and high entropy of the unfolded ensemble of states, the "coil" metastable set contains the largest number of structures. Interestingly, the helix metastable state was also found to be structurally heterogeneous, consisting of the completely helical form and several partly folded conformers which interconvert at a time scale faster than global folding. The intermediate states contain the fewest structures, have lowest populations and have the shortest lifetimes. As the number of considered metastable states increases, more intermediates and more folding paths appear in the coarse-grained models. One of these intermediates corresponds to the transition state for folding, which involves an "off-center" helical region over residues 11-16. The simulation data further suggest that the experimentally observed fast kinetic time scale should be assigned to correlated breaking/formation of blocks of several adjacent helical hydrogen bonds. The same computational analysis was also applied to a 13-microsecond molecular dynamics trajectory of the peptide with the neutral form of its histidine residue, corresponding to a higher pH. The loss of the histidine proton induces significant changes in the free energy landscape. This form has a higher helix content than the protonated peptide, in accord with experimental observations. Additionally, the kinetic network and folding pathway are also markedly different.



CNBCh Research Group:  
**Ecology and Toxicity of Cyanobacteria  
headed by Prof. Iwona Jasser**

## Prof. Gkelis Spyridon

### Activity at Home University:

Assistant Professor in the School of Biology, Aristotle University of Thessaloniki

**Research field:** Bioinformatics and Biodiversity of photosynthetic organisms. Spyros Gkelis is the head of the Cyanolab research group where he and his team investigate the diversity and genomics of aquatic microorganisms, how species interact with each other and with the abiotic environment, what drives their secondary metabolite production. In addition to doing research he teaches undergraduate/Master's courses in Biodiversity, Phycology, Bioinformatics, Applied Microbiology, Aquacultures and serves in the board of several MSc Programs.

### Activity at CNBCh UW:

Presented a seminar and was developing joint experimental project on thermophilic cyanobacteria with Prof. Iwona Jasser.

**University:** [University of Thessaloniki](#)

**Country:** Greece

### Date of stay:

24 August – 4 September 2020

### Prof. Iwona Jasser about cooperation:

During the stay of the prof. Spyros Gkelis in CNBCh at Warsaw University we had

1) lecture of prof. Spyros Gkelis (in a mixed version - stationary and remote) on 25.08.2020. The lecture was titled: "Toxic cyanobacteria in Europe: threats, challenges, opportunities"

2) workshop (in a mixed version – stationary and remote) on 25 and 26<sup>th</sup> 08.2020. The workshop concerned thermophilic cyanobacteria and was titled: "The morphology, phylogeny and biogeography of thermophilic strains of cyanobacteria"

3) The study part of the visit concerned work on results for a joint manuscript on thermophilic cyanobacteria.

In the lecture and workshop were researchers and students from the Faculty of Biology UW and from other universities in Poland (Łódź, Poznań, Gdańsk).

**Effects:** The main result of the visit is the manuscript titled: "Cyanobacteria hot pursuit: Characterisation of cyanobacteria strains, including novel taxa, isolated from geothermal habitats from different ecoregions of the world". We presently finish preparations of the manuscript and the manuscript will be submitted still this month. After the submission we plan to develop further collaboration on thermophilic cyanobacteria and apply together for a joint project. This however has not yet an apparent application deadline. Another effect of the visit are plans for Erasmus visits of our PhD students which due to the pandemic were on hold for some time.

# LECTURE

## Prof. Spyros Gkelis

Department of Botany, Faculty of Biology, Aristotle University of Thessaloniki

### Toxic cyanobacteria in Europe: threats, challenges, opportunities

**DATE:** Tuesday, 25 August 2020 | 11.00 **VENUE:** CNBCh, seminar room 0.36

#### ABSTRACT:

Toxigenic cyanobacteria are one of the major health risks associated with water resources, in Europe and beyond. The continuing eutrophication of many aquatic ecosystems and water resources in Europe is causing concern because the deterioration of water quality and Harmful Algal Blooms of cyanobacteria (cyanoHABs) threaten human, animal, and environmental health. Cyanobacterial blooms occur when algal densities exceed baseline population concentrations. Global changes resulting from human impacts, such as over-enrichment of waterways are major drivers of cyanoHAB proliferation and persistence. Moreover, there is increasing evidence that both direct and indirect effects of global warming will favor and intensify cyanobacterial blooms.

Cyanobacteria are prolific bioactive secondary metabolite producers, which can affect the activity of cellular enzymes, interfere with signaling pathways in cells, cause apoptosis of tissues, and lead to a range of lethal and sub-lethal effects in plants, invertebrates, and vertebrates, including humans. These metabolites include a wide range of potent toxins (cyanotoxins) with adverse health effects on humans and animals exposed e.g. via drinking water, aquaculture and recreation. Odorous metabolites affect the smell and flavor of aquatic animals and drinking waters. More than 150 known bioactive compounds classes produced by cyanobacteria have been elucidated up to know. This diversity in secondary metabolites arises from the cyanobacterial capacity to integrate both non-ribosomal peptide synthetases with polyketide synthases in their biosynthetic pathways. The biosynthetic logic underpinning this chemical diversity is slowly being unraveled with traditional and new tools such as metabolomics and comparative genomics and high resolution mass spectrometry, establishing links between the known chemical diversity of natural products and genomes. Nonetheless, the variety, the biosynthetic, and evolutionary routes of secondary metabolites cyanobacteria can produce or the worldwide expansion of certain species acquiring adaptive mechanisms are still far from being solved.

Over the past decades it has become evident that marine, terrestrial and freshwater cyanobacteria, in order to adapt in diverse environments, produce a wealth of natural products, in addition to cyanotoxins, with over 1100 natural products already known. Many of these products, have interesting biological activities including antimicrobial, anticancer, anti-inflammatory, antioxidant compounds, antifouling agents and nutraceuticals rendering cyanobacteria bio-synthetic factories holding the recipes for a plethora of pharmacologically and biotechnologically useful metabolites. Overall, cyanobacteria continue to be an excellent source of new and exciting discoveries.

**VISITING  
PROFESSOR  
PROGRAMME**

**Warsaw, 2021**