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KSUPS`17

Gdańsk
4-7 September 2017

XII National Symposium of the Synchrotron Radiation Users

Organized by Polish Synchrotron Radiation Society in cooperation with Gdańsk University of Technology, Gdańsk Poland

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Monday, 4 September 2017 PROGRAMME

8^{00}-10^{00}	Registration		
10^{00}-10^{10}	Opening Address by **Maciej Kozak** (PSRS Chair) and **Jacek Namieśnik** (Rector of the GUT)		
10^{10}-10^{55}	L-01	**Marek Stankiewicz**	National Synchrotron Radiation Centre SOLARIS - current status and future development
10^{55}-11^{15}	O-01	**Robert Nietubyć**	A test linear accelerator for FEL development
11^{15}-11^{45}	Coffee Break		
	Topical session: X-ray lasers and synchrotron methods		
11^{45}-12^{15}	L-02	**Jakub Szlachetko**	Nonlinear interaction of X-rays with matter
12^{15}-12^{45}	L-03	**Ryszard Sobierajski**	Polish involvement in X-ray Free Electron Lasers
12^{45}-13^{05}	O-02	**Karol Janulewicz**	Quantum X-ray lasers pumped by XFEL radiation
13^{05}-13^{25}	O-03	**Robert Mroczka**	Micro- X-Ray fluorescence spectrometer with X-ray single bounce gold capillary optics for light element analysis
13^{30}-15^{00}	Lunch		
	Topical session: Spectroscopy of gas phase and plasma		
15^{00}-15^{20}	O-04	**Małgorzata Śmiałek**	Electronic state spectroscopy of small ether molecules in the gas phase
15^{20}-15^{40}	O-05	**Tomasz Wąsowicz**	Inner-shell photoexcitation and fragmentation of isoxazole molecules at the K edges
15^{40}-16^{00}	O-06	**Andrzej Bartnik**	Photoionized plasmas induced by extreme ultraviolet or X-ray intense pulses
16^{00}-16^{30}	Coffee Break (Welcome Party)		
16^{30}-19^{00}	**Poster session**		

Tuesday, 5 September 2017

	Topical session: Structural properties – photoemission spectroscopy		
9^{00}-9^{30}	L-04	**Piotr Dziawa**	Photoemission spectroscopy of topological crystalline insulators (Pb,Sn,Mn)Se
9^{30}-9^{50}	O-07	**Zbigniew Klusek**	Towards hybride systems - ARPES and STM/STS investigations of graphene, transition metal dichalcogenides and topological insulators
9^{50}-10^{10}	O-08	**Yevgen Syryanyy**	Usefulness of photoelectron spectroscopy to study surfaces and interfaces: selected examples
10^{10}-10^{30}	Coffee Break		
	Topical session: Structural properties – X-ray diffraction		
10^{30}-11^{00}	L-05	**Katarzyna Jarzembska**	Tracing structure-property relationships in crystals of selected photoactive copper(I) coordination complexes
11^{00}-11^{30}	L-06	**Radosław Kamiński**	High-pressure single-crystal X-ray diffraction studies of organic-inorganic compounds at ID15B beamline at ESRF
11^{30}-12^{00}	L-07	**Maciej Jankowski**	Synchrotron X-ray diffraction methods for surface characterization
12^{00}-12^{20}	O-09	**Maciej Zieliński**	CLD - atomic Column Length Distribution and Crystal Lattice Dynamics of supported gold catalysts. The key to understand their catalytic activity
12^{30}-14^{00}	Lunch		
14^{00}-19^{00}	Excursion		

Wednesday, 6 September 2017

Topical session: Structural properties – X-ray spectroscopy

9^{00}-9^{30}	L-08	**Krystyna Ławniczak-Jabłońska**	X-ray absorption for characterisation of new materials – the overview of the accessible unique information
9^{30}-9^{50}	O-10	**Joanna Stępień**	Determination of oxygen vacancy limit in Mn substituted YSZ ceramics
9^{50}-10^{10}	O-11	**Paweł Rejmak**	Determining the structure of novel bioactive Cu(II)-thiourea complexes by combined XAFS spectroscopy, laboratory techniques and DFT calculations
10^{10}-10^{30}	Coffee Break		

Topical session: Synchrotron methods for biology and medicine

10^{30}-11^{00}	L-09	**Marcin Nowotny**	Structural Biology
11^{00}-11^{20}	O-12	**Weronika Andrzejewska**	Specification of gene carriers based on ammonium gemini surfactants and siRNA enhancing DMPK gene in type 1 myotonic dystrophy (DM1)
11^{20}-11^{40}	O-13	**Diana Kalinowska**	Molecular structure investigation of coumarin complexes with Cu ions
11^{40}-12^{00}	O-14	**Joanna Czapla-Masztafiak**	X-ray spectroscopy for analysis of metal anti-cancer complexes and their interaction with biomolecules
12^{00}-14^{00}	Lunch		

Topical session: Numerical methods and simulations for spectroscopy

14^{00}-14^{30}	L-10	**Marta Łabuda**	Fragmentation of molecules using quantum chemistry methods
14^{30}-15^{00}	L-11	**Julien Guthmuller**	Calculation of resonance Raman and photoelectron spectra of molecules using quantum chemistry methods
15^{00}-15^{20}	O-15	**Pavlo Konstantynov**	Application of molecular dynamics simulations to interpret X-ray absorption spectra
15^{20}-15^{40}	O-16	**Marek Brancewicz**	Monte Carlo simulations of multiple scattering in Compton spectroscopy
15^{40}-16^{00}	Coffee Break		
16^{00}-19^{00}	General Assembly of the Polish Synchrotron Radiation Society		
19^{30}-	Conference Dinner ("Nad Potokiem" Restaurant, Gdańsk-Jelitkowo)		

Thursday, 7 September 2017

Special session: ESRF – present and future

9^{00}-9^{30}	L-12	**Harald Reichert**	ESRF: Overview, EBS project, new beamlines and research opportunities
9^{30}-10^{00}	L-13	**Pieter Glatzel**	Spectroscopy at the ESRF
10^{00}-10^{30}	L-14	**Andy Fitch**	X-ray diffraction and scattering opportunities at ESRF
10^{30}-11^{00}	O-17	**Joanne McCarthy**	How to prepare and submit project to ESRF
11^{00}-11^{30}	Coffee Break		

Special session: SOLARIS – present and future

11^{30}-12^{00}	L-15	**Adriana Wawrzyniak**	Solaris Synchrotron – from the start up to first experiments
12^{00}-12^{30}	L-16	**Jacek Kołodziej**	Angle-resolved Photoelectron Spectroscopy at National Center for Synchrotron Radiation SOLARIS
12^{30}-13^{00}	L-17	**Marcin Zając**	Status and first results of the PEEM/XAS beamline commissioning process
13^{00}-13^{30}	L-18	**Jacek Szade**	Future beamlines at SOLARIS
13^{30}-13^{50}	O-18	**Alicja Górkiewicz**	SOLARIS user office
13^{50}-14^{00}	Closing Remarks		
14^{00}-16^{00}	Lunch		

L-01 **Monday, 04.09., 10^{10} - 10^{55}**

National Synchrotron Radiation Centre SOLARIS - current status and future development

Marek Stankiewicz[1]*

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National Synchrotron Radiation Centre SOLARIS in Kraków is the most modern and largest multidisciplinary research facility in Poland. The Centre was built between 2010 and 2015. The investment was co-financed by the European Union with funds from the European Regional Development Fund, as part of the Innovative Economy Operational Programme for 2007-2013.

SOLARIS has been built using the groundbreaking design of magnetic double bend achromats developed at MAX-lab facility in Lund, Sweden, resulting in outstanding properties of generated synchrotron light which places SOLARIS firmly at the cutting edge of devices of this type. SOLARIS synchrotron operates at 1.5GeV energy with up to 500mA stored electron beam. It is powered by 600MeV S-band linac.

SOLARIS can provide synchrotron radiation for up to 18 beamlines from bending magnets and insertion devices. Within the scope of the project budget already two beamlines have been constructed.

As a strategic investment for the development of science, SOLARIS has been included on the Polish Roadmap for Research Infrastructures.

The presentation will provide a brief history of the project and describe configuration and key parameters of the SOLARIS facility. However the presentation will focus on the current status and plans for the future development of SOLARIS and its offer for researchers.

L-02 **Monday, 04.09., 11^{45} – 12^{15}**

Nonlinear interaction of X-rays with matter

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X-rays have long been used to explore the electronic and structural properties of all forms of matter, using sources as varied as X-ray tubes to accelerator-based storage rings. X-ray methods have evolved over decades to become specialized tools for a broad range of investigations, with techniques ranging from X-ray scattering through X-ray spectroscopy to X-ray tomography. In general these methods all rely on X-ray measurements that depend linearly on the number of incident X-ray photons. With the advent of X-ray free electron lasers (XFELs), the ability to reach extremely high photon numbers in ultrashort pulse durations has resulted in a paradigm shift in our ability to observe nonlinear X-ray signals. This enormous increase in peak power (pulse energy/pulse duration) has been a double-edged sword, with new and exciting techniques being developed but at the same time well-established techniques proving unreliable [1-3]. This requires a fundamental change in our approach to X-ray science at FELs, since this nonlinear regime is a largely unexplored area, making it hard to predict not only when to expect nonlinear contributions to a measurement, but also to understand the very nature of this response [4-6].

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[1] K. Tamasaku *et al.: Nature Photon.* **8** (2014) 313.
[2] N. Rohringer *et al.: Nature* **481** (2012) 488.
[3] M. Beye *et al.: Nature* **501** (2013) 191.
[4] S. M. Vinko *et al.: Nature* **482** (2012) 59.
[5] T. E. Glover *et al.: Nature* **488** (2012) 603.
[6] J. Szlachetko *et al.: Scientific Reports* **6** (2016) 33292.

L-03 **Monday, 04.09., 12^{15} - 12^{45}**

Polish involvement in X-ray Free Electron Lasers

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From the birth of a new type of light source, the short-wavelength free electron lasers, Polish scientists were involved both in work at its technical development and its use for scientific research. Short-wavelength FELs provide laser-like pulses of radiation (including high intensity, femtosecond pulse duration, high spatial and partial temporary coherence, polarization) but in the spectral range of extreme ultraviolet and x-ray, unavailable for laser sources. In my early studies at the first short-wavelength FEL - TTF1 FEL - I investigated the structural phase transitions in thin films that are crucial for the construction of optics for the intense XUV and X ray sources. Over time, the FEL scientific community in Poland has grown and currently it consists of several research groups gathered in the XFEL-Polska consortium. One of the main aims of this initiative is to share the expertise of how to prepare and perform the experiments, and spread the knowledge in experimental opportunities and challenges at FELs by training the new generation of Polish FEL users. In particular we plan to cooperate at joint research projects at the newest source, the European XFEL, in a broad range of scientific disciplines – physical chemistry, material sciences, structural biology and high energy density physics. During my talk I will present my personal perspective on the history of short-wavelength FEL sources and discuss some of the research plans of the XFEL-Polska consortium.

Acknowledgements: This work was supported by the international project co-financed by Polish Ministry of Science and Higher Education, Grant Agreement 2819/7.PR/2013/2.

L-04 **Tuesday, 05.09., 9^{00} – 9^{30}**

Photoemission spectroscopy of topological crystalline insulators (Pb,Sn,Mn)Se

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In recent years a new very hot topic in solid state physics emerged, i.e. the discovery of topological insulators (TIs) – new quantum materials [1]. It has been predicted theoretically, that in topologically nontrivial phase TIs are band insulators with opposite parity in the band structure and they host surface states (SS) with metallic-like conductivity (Dirac SS). The topological protection of SS comes from time-reversal symmetry and strong relativistic (spin-orbit) effects. Experimental findings validated the unique features of these materials, i.e. linear energy-momentum dispersion of the SS with odd number of Dirac cones and specific helical spin texture which means that they are robust against back-scattering on non-magnetic ions.

In 2011 Liang Fu proposed a new class of topological materials so-called topological crystalline insulators (TCIs) where topological protection is due to a (110) mirror-plane symmetry of the rock-salt crystal structure, and exhibits an even number of Dirac cones [2]. Tin telluride was predicted to be a representative TCI material. However substitutional solid solutions, such as $Pb_{1-x}Sn_xSe$ also belong to this class. Transition to the topologically non-trivial state in TCIs can be controlled by changes of the temperature [3], chemical composition of an alloy [3], by applying hydrostatic pressure [4] or by crystal lattice distortion [5].

The experimental studies of the electronic structure of the TCIs presented here have been performed using angle-resolved photoemission spectroscopy (ARPES) in the wide ranges of both chemical compositions and temperatures. This allows us to built x-T topological phase diagram. The (001) and (111) high symmetry topological surfaces of the $Pb_{1-x}Sn_xSe$ were realized by cleaved bulk monocrystals [3] and in-situ deposition of the layered structures [6], respectively. Spin-resolved photoemission spectroscopy (SRPES) revealed spin texture in a full agreement with the tight-binding calculations.

From previous investigations a new approach arose, i.e. possibility of controlling the TCI transition by the band gap engineering. In order to corroborate this concept as well as to verify topological protection in TCI the manganese ions were introduced into the host matrix. The Mn partially substituting the host cation sites in these compounds changes both the energy gap and lattice parameter and constitutes a magnetic impurity. The increase of Mn content in $Pb_{1-x-y}Sn_xMn_ySe$ lowers the temperature of TCI transition compared to the analogue ternary non-magnetic $Pb_{1-x}Sn_xSe$. Density functional theory calculations qualitatively reproduce the experimental findings. $Pb_{1-x-y}Sn_xMn_ySe$ exhibit a paramagnetic ordering, and Mn is in 2+ charge state and carries spin-only S=5/2 local magnetic moment. The first observations lead to conclusion that magnetic ions do not destroy Dirac-like surface states. The inspection of the spin texture shows similar helical pattern for TCIs without magnetic impurities.

Acknowledgements: This work has been partially supported by the research projects 2014/15/B/ST3/03833 and 2016/21/B/ST5/03411 financed through the National Science Centre (Poland).

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L-05 **Tuesday, 05.09., 10^{30} – 11^{00}**

Tracing structure-property relationships in crystals of selected photoactive copper(I) coordination complexes

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One of the most important current areas in chemistry is developing new materials that are able to respond rapidly and reliably to changes in local environment, and send out signals that let us know what is happening. Therefore, chemical compounds exhibiting specific photoactive properties, either in solution or, even more importantly, in the solid state, are among the most desired materials nowadays. Especially interesting here are luminescent coordination complexes of transition metals, which have versatile applications in solar-energy conversion and other fields ranging from molecular electronics and photocatalysts to light-emitting devices (LEDs) and biolabels. It is, thus, of high importance to sensibly control optical properties of such materials at the molecular level, so as to apply this knowledge to generate materials with particular properties across all the size scales from molecules to bulk materials, relevant for specific applications. In this respect, information on structural changes and charge transfer (CT) occurring on electronic excitation is essential for rational design of new materials. Such information is now becoming available through time-resolved (TR) X-ray absorption and photocrystallographic techniques. In the current presentation we shall focus on the latter method which takes advantage of the powerful X-ray beam produced at synchrotron sources.

We will describe the time-resolved laser-pump / X-ray probe Laue experiments and show our latest results obtained using this technique at APS (Argonne, USA) and ESRF (Grenoble, France) for selected Cu^{I} coordination complexes.[1,2] The choice of such systems has been dictated by the fact that coordination complexes of Cu^{I} are often characterised by rich electronic and luminescent properties and are cheaper and usually less toxic than heavy-metal-containing compounds (*e.g.*Ru^{II} or Ir^{III}). The photocrystallographic and spectroscopic analyses will be supplemented by theoretical modelling.

Acknowledgements: KNJ thanks the SONATA grant (2014/15/D/ST4/02856) of the National Science Centre in Poland for financial support. The authors gratefully acknowledge the Wroclaw Centre for Networking and Supercomputing (grant No. 285) for providing computational facilities. Some part of this research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357. Use of BioCARS was also supported by the National Institute of General Medical Sciences of the National Institutes of Health under grant number R24GM111072. The content is solely the responsibility of the authors and does not necessarily represent the official views of the National Institutes of Health. Time-resolved set-up at Sector 14 was funded in part through a collaboration with Philip Anfinrud (NIH/NIDDK). This research has been realised within the GUP-46291 proposal number. Some experiments were performed on beamline ID09 at the European Synchrotron Radiation Facility (ESRF) (Grenoble, France) (beamtime proposal numbers: CH-4536,4935,4934,4744).

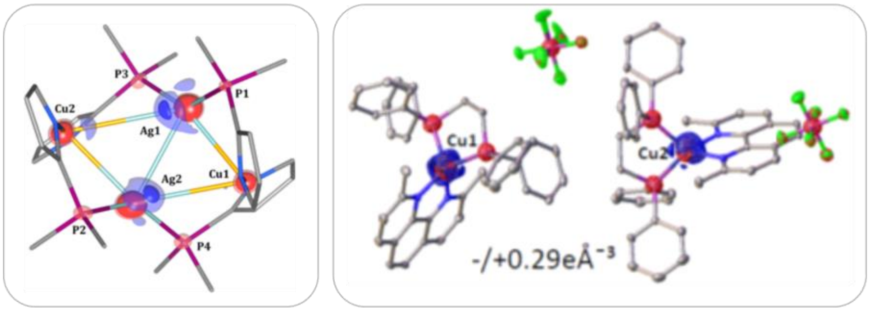

Figure 1. Example photodifference maps.

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L-06 **Tuesday, 05.09., $11^{00} – 11^{30}$**

High-pressure single-crystal X-ray diffraction studies of organic-inorganic compounds at ID15B beamline at ESRF

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High pressure studies of materials constitute an important field of research. The high-pressure phases, often exhibiting unique properties, are formed in geological processes (e.g. new minerals), pharmaceutical formulations (e.g. while preparing pills), or when various materials are exposed to extreme conditions on purpose (e.g. shock waves). Hence, the detailed knowledge of the materials' structure is indispensable to understand, and later to potentially sensibly control, their behaviour and function. In this respect high-pressure single-crystal X-ray diffraction experiments provide full picture of material's structure with atomic resolution. This, in turn, allows to establish a 'standard of gold' as far as high-pressure phase transitions, etc., are concerned. Consequently, in this contribution we will describe our recent studies on two types of organic-inorganic materials exhibiting interesting spectroscopic properties. In both cases the high-pressure data collection has been done at the (partially new) ID15B beamline at the ESRF facility.

A boron- containing compound, which undergoes some phase transition in the solid state at elevated pressure, constitutes the first presented case. Out of many solvatomophic structures it forms, the structure containing tetrahydrofuran (THF) undergoes the high-pressure phase transition. In the new phase the THF molecules are rotated.

The second study is dedicated to a rhodium complex, namely $LRh(CO)_2$ (L = 3-benzoylacecate), which exhibits chain substructures based on Rh...Rh interactions propagating along the *Y*-axis direction. Temperature does not have a significant impact on the structural parameters (except for the less obvious unit cell choice in the case of the high temperature structure). In turn, the application of high pressure leads to a phase transition, in which the Rh...Rh chains differentiate noticeably. As a result the structure becomes modulated and has to be treated within a super-space approach. In addition, the whole crystal needs to be treated with the multi-phase model due to the incomplete phase change.

Acknowledgements: High-pressure experiments were conducted at the ID15B beamline of the ESRF facility (Grenoble, France) (proposal no.: CH-4903). We thank the Wrocław Centre for Networking and Supercomputing for computational facilities (grant no.: 285). K.N.J. would like to thank SONATA grant (2014/15/D/ST4/02856) from the National Science Centre in Poland for financial support. The in-house X-ray diffraction experiments were carried out at the Department of Physics, University of Warsaw, at the Rigaku Oxford Diffraction SuperNova diffractometer, which was co-financed by the European Union within the European Regional Development Fund (POIG.02.01.00-14-122/09).

L-07 **Tuesday, 05.09., $11^{30} – 12^{00}$**

Synchrotron X-ray diffraction methods for surface characterization

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Surface X-ray diffraction (SXRD) allows the exact structure determination of surfaces, interfaces, and thin films. In comparison with other diffraction surface sensitive methods, like electron or helium atom diffraction, the main advantage of SXRD is the capability to penetrate deeply into matter allowing the investigation not only of the surface structure, but also the structure of the sub-surface region. The high x-ray penetration depth allows to perform *operando* study of materials at conditions ranging from ultra-high vacuum (UHV) to high pressure or in a liquid environment. The high brilliance synchrotron source of x-rays is a necessity for such kind of experiments, as the diffraction signal from the surface is few orders of magnitude lower than from the bulk, and the reciprocal space resolution, corresponding to the periodicity of tens of nanometers in the real space, can be achieved thanks to the spatial coherence of the x-ray beam.

SXRD, together with grazing incidence small angle scattering and wide angle scattering (GISAXS and GIWAXS, respectively), is frequently used in the operando characterization of single crystal surfaces and surface supported nanoparticles at catalytic near-ambient conditions. This allows to obtain information about their crystallographic structure, morphology, and monitoring of their structural changes in a real-time. SXRD is widely-used for resolving the structure and the growth dynamics of thin layers of metals, oxides, semiconductors, molecular films, nanocrystals superlattices, and nanometer-sized nanoparticles.

The ID03 beamline is dedicated to SXRD at the ESRF, the European Synchrotron, which offers ideal conditions for the fast characterization of surfaces and interfaces in different environments. This is possible thanks to the high brilliance synchrotron X-ray beam, the use of sensitive large-area 2D detectors, and the recently developed software for the fast analysis of collected data. Its access is open to the European community.

The aim of this contribution is to present the ID03 beamline, its experimental opportunities, and provide some examples focused on the structural determination of single crystal (bi)metallic surfaces under catalytic *operando* conditions, real-time characterization of topologically insulating thin films growth, and their solid-liquid phase transition.

L-08 **Wednesday, 06.09., 9^{00} – 9^{30}**

X-ray absorption for characterisation of new materials – the overview of the accessible unique information

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The characteristic features of the x-ray absorption spectra (XAS) are elemental selectivity, and the ‘finger print’ of local atomic order and chemical bounding. Therefore, XAS can be applied to study elemental, chemical and the phase heterogeneity in materials. These information are of great interest in characterization of new materials being nowadays mostly composite or/and nano granular materials. Several examples of XAS investigation of heterogeneous materials will be presented.

The application of the analysis of near edge structure (XANES) for solving the phase heterogeneity problem will be presented for composite material used in tools production and artworks [1, 2]. The most popular method for quantitative analysis of the content of different chemical compounds of a given element is the least squares linear combination (LC). The method is simple and easy to implement. It uses the least-squares algorithm to fit the sum of a given number of reference spectra to an experimental spectrum. The LC method and the modern detection allowed e. g. to estimate the nature and distribution of secondary Cr compounds and quantitatively determining their abundance in two paint micro-samples taken from artworks by Vincent van Gogh [2].

The use of XAS to address the problem of chemical heterogeneity will be demonstrated in the cases of natural minerals [3]. The alternative method to check if all considered references are necessary needed or are sufficient to fit the spectrum under consideration is the principal component analysis (PCA). This method will be briefly introduced. It has become nowadays routine to collect hundreds of spectra on a single sample e.g. in function of time. For analysis of such a data the LC requires reference spectra and PCA often provides mixed components that are hard to interpret. In such a case the multivariate curve resolution with alternating least squares fitting (MCR-ALS) can be used as a method to separate constituents from XAS data.

The effectiveness of the analysis of extended x-ray fine structure (EXAFS) will be shown with regard to the problem of doped elements location in the crystalline matrix. The case of the classical GaMnAs semiconductor will be considered. The fraction of Mn atoms located in interstitial and substitutional position will be assessed in the case of as grown samples, together with distribution of Mn atoms amid the cubic and the hexagonal inclusions after post growth annealing [4]. Moreover, calculated XAS spectra for different location of atoms in a given crystal structure show significant differences. The quantitative comparison of the calculated model spectra with measured spectra can thus be a quick homogeneity checking procedure. The x-ray transitions preserve the electron spin, therefore are magnetic sensitive. This feature is named X-ray magnetic circular dichroism (XMCD). This kind of x-ray absorption study also provided unique information. Although, the best mode of XMCD detection is the transmission for majority of reported in the literature experiments the total electron yield (TEY) and total fluorescence yield (TFY) were applied. These two detection modes differ also in the examined depth and can provide different result in the case of inhomogeneous samples: e.g. for sample containing the cubic GaMnAs and hexagonal MnAs nano-clusters the signal significantly differs (Fig.1). Several nano-granular materials studies will illustrate usefulness of XMCD.

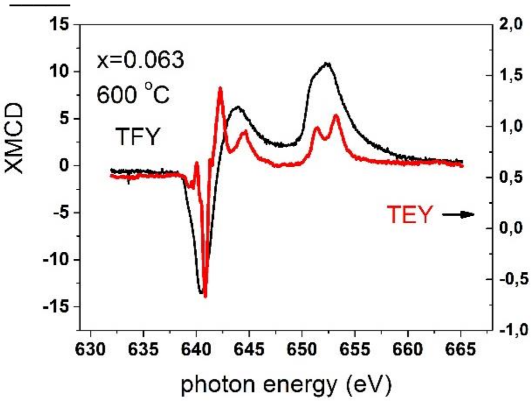

Figure 1. XMCD signal for TEY and TFY modes of detection.

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L-09 **Wednesday, 06.09., 10^{30} – 11^{00}**

Structural biology

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Structural biology provides information on the architecture of biological molecules, in particular proteins and nucleic acids, at the level of individual atoms. This allows us to understand not only their chemical structure, but also the details of their mechanism of action in physiological and pathological processes. For most of the history of structural biology it was dominated by one method - protein crystallography. In this method, microcrystals of the studied molecule are obtained and the X-ray diffraction experiment is carried out on these crystals. At this stage it is crucial to use a synchrotron X-ray source. From the diffraction pattern, the spatial distribution of electrons in the crystal can be calculated, and hence the position of the atoms of the molecule can be determined.

In the last few years a revolution in structural biology has taken place due to the development of modern high-resolution electron microscopy methods at cryogenic temperatures (cryo-EM). Traditional cryo-EM has routinely been able to achieve a resolution of about 10 Å, too low to determine the atomic model of the molecule. Thanks to the construction of very fast and sensitive cameras, so-called “direct detectors” and the development of appropriate software, it has become possible to obtain structures with a resolution comparable to crystallography - in the range of 2-3 Å. The use of modern cryo-EM has led to the identification of groundbreaking and previously inaccessible structures such as eukaryotic ribosomes, spliceosomes or membrane proteins.

As examples of research conducted using both crystallography and electron microscopy, our structural studies of proteins involved in the repair of genetic material will be presented.

L-10 **Wednesday, 06.09., 14^{00} – 14^{30}**

Fragmentation of molecules using quantum chemistry methods

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Since several years the aim of our work is to investigate and understand the mechanism of charge transfer and fragmentation processes occurring in collisions between ions and atoms or molecules [1-4]. To achieve this goal we merge the state-of-the-art quantum chemical and dynamical techniques and apply them to a series of collision systems. Especially, we use and develop modern numerical tools, allowing for an investigation of both processes in the ultrafast femtosecond (1 fs=10^{-15}s) time scale. Such studies are of high relevance in the understanding of the action of ionizing radiation, namely radiation damage in DNA, cell killing and repairing. Ion beam cancer therapy and, in general, cancer research, may benefit from these capabilities. As an example of the application of our methodology we selected neutral and ionized furan molecule, which belong to the family of ring structures that are analogous to the deoxyribose building block of the DNA helix. Therefore, this molecule can serve as a model system for track simulations in biological medium [3,4].

As a first step, to determine the structure of the molecule, the results of the electronic properties and lowest excited states obtained by *ab initio* (HF, MP2, CASSCF, EOM-CCSD), propagator (P3, OVGF) and density functional theory (with B3LYP functional) methods will be presented. The accuracy of the methods is estimated with experimental and theoretical results given in literature. To interpret the fragmentation mechanisms and to determine accessible products of dissociation we performed calculations of minima and transition states on the potential energy surfaces using Density Functional Theory. We applied Atom-Centered Density Matrix Propagation method to study dynamics of the process. We present the results obtained for the cases of 5-30 eV internal energy being applied to the system and discuss the different mechanisms arising from the fragmentation. The general fragmentation dynamics of the system is dominated by the opening of the furan ring and H migration and its transfer. The most frequent channel involves production of acetylene by direct C-C bond cleavage. For singly-ionized furan, the most abundant channels include production of formyl radical (CHO*), cyclopropenyl ($C_3H_3^+$) and $C_3H_4O^+$ cations with H atom out of dehydrogenation process. A comparison of experimental data, i.e. photoelectron photoion coincidence spectroscopy vs. theoretical results will also be given.

Acknowledgements: We gratefully acknowledge financial support from COST Action CM1204 "XUV/X-ray light and fast ions for ultrafast chemistry" and Erasmus Plus programme (M.Ł). Calculations were performed at Wroclaw Centre for Networking and Supercomputing, Centro de Computación Científica in Madrid, Universitätsrechenzentrum at Friedrich Schiller University in Jena.

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L-11 **Wednesday, 06.09., $14^{30} – 15^{00}$**

Calculation of resonance Raman and photoelectron spectra of molecules using quantum chemistry methods

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Electronic and vibrational spectroscopies, like UV/Vis absorption, photoelectron and resonance Raman (RR), are useful techniques to provide information on structures and properties of molecules in their ground and excited states. Moreover, quantum chemistry methods are able to accurately predict the energies, the geometries, the vibrational modes and frequencies, as well as the electronic properties of the molecular states. Therefore, the simulation of spectra, using quantum chemistry methods, can help in the interpretation of experimental data as well as in the design of new compounds for specific applications, as for example, in dye-sensitized solar cells or as photocatalysts for hydrogen generation. Additionally, the calculation of absorption, photoelectron or RR intensities and their comparison with precise experimental data offers an opportunity to assess the ability of standard quantum chemistry methods to predict molecular properties.

In this contribution, theoretical absorption and RR spectra are presented for the organic molecule of Rhodamine 6G and for a Ruthenium-Palladium supramolecular photocatalyst [1,2]. The calculations are performed with density functional theory (DFT) and with time-dependent DFT (TDDFT). The obtained results are compared to experimental data and their accuracy is discussed. In particular, the importance of Franck-Condon (FC) and Herzberg-Teller (HT) vibronic couplings is considered. Additionally, the first ionization energy and associated photoelectron spectrum are calculated for a series of small esters [3,4]. These calculations are realized with the wavefunction-based methods, second-order Møller-Plesset perturbation theory (MP2) and coupled-cluster. In particular, the effects of Duschinsky couplings are investigated on the photoelectron intensities.

Acknowledgements: The author is grateful to the Narodowe Centrum Nauki (Project No. 2014/14/M/ST4/00083) for financial support. The calculations have been performed at the Universitätrechenzentrum of the Friedrich-Schiller University of Jena.

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L-12 **Thursday, 07.09., $9^{00} – 9^{30}$**

ESRF: Overview, EBS project, new beamlines and research opportunities

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L-13 **Thursday, 07.09., $9^{30} – 10^{00}$**

Spectroscopy at the ESRF

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The experimental requirements for X-ray spectroscopy critically depend on the problem that the researcher wishes to study. The ESRF offers a large number of experimental stations each optimized for specific applications and thus meets the needs in most fields of natural sciences. Bending magnet (BM) beamlines provide ideal conditions for high quality X-ray absorption experiments in transmission or fluorescence detection mode while insertion device (ID) beamlines push the limits with respect to beam size, total photon flux, time- and energy-resolution. X-ray absorption spectroscopy with beamsize down to a few hundred nanometers can be performed on ID21. An energy dispersive X-ray optics layout on ID24 allows recording of a transmission absorption spectrum with an X-ray pulse from only one electron bunch providing time-resolution in the nano-second range. Detection of X-ray absorption dichroism requires highest possible measurement accuracy and full control of the X-ray polarization as provided on ID12. Photon-in/photon-out spectroscopies such as Resonant Inelastic X-ray Scattering (RIXS), X-ray Emission Spectroscopy (XES) and X-ray Raman Spectroscopy (XRS) are available on ID20, ID26, ID32, FAME-UHD and ROBL covering the soft to hard X-ray range [1–3]. In a very recent development, the ESRF now offers XES combined with picosecond time-resolution on ID09.

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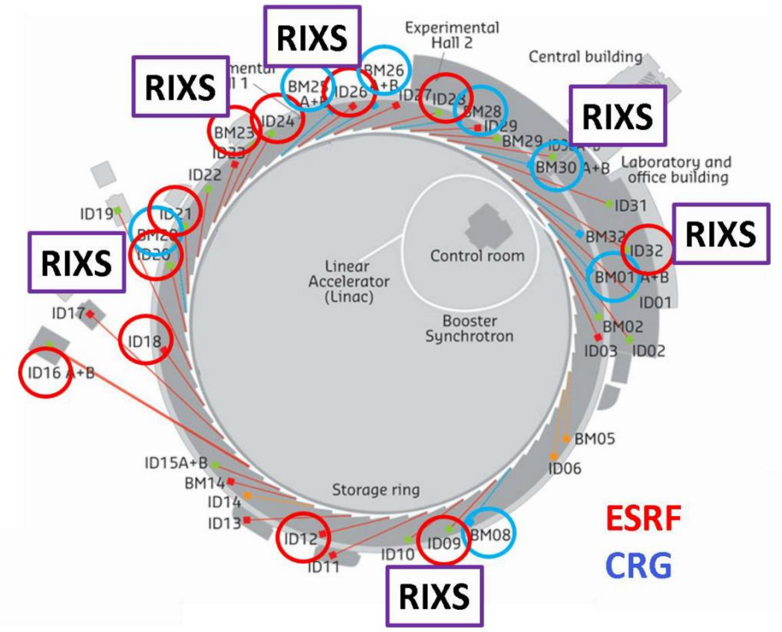

Figure 1. X-ray spectroscopy beamlines at the ESRF.

L-14 **Thursday, 07.09., 10^{00} – 10^{30}**

X-ray diffraction and scattering opportunities at ESRF

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The ESRF has several beamlines, particularly in the Structure of Materials group, that between them allow X-ray diffraction and scattering experiments over a wide energy range, from the relatively soft, 6 keV, through to the distinctly hard, in excess of 500 keV at the upper limit.

ID11, the Materials Science Beamline, was one of the first to operate at the ESRF, and, following several upgrades, is dedicated to moderate to high energy powder or single-crystal diffraction and/or imaging studies of a variety of systems of interest for their physical, mechanical, or chemical properties. Very high spatial (<100 nm) and time (1 ms) resolution are available.

ID15A, Materials Chemistry and Materials Engineering, newly refurbished as part of phase I of the ESRF upgrade, is a highly versatile instrument that allows a wide range of in-situ measurements in the areas of materials chemistry, catalysis, and metallurgy, among other areas. It is equipped with a hard-energy, CdTe-based Pilatus 2M photon-counting pixel detector providing rapid counting and outstanding data quality.

ID22 is the high resolution powder diffraction beamline. As well as providing high resolution data of high accuracy, the beamline was recently equipped with a large 2d medical imaging detector for complementary measurements, for samples where angular resolution is less of a priority, including data for pair-distribution function (PDF) analysis. A wide range of sample environments is available, allowing measurements from 4 K to 1600°C for capillary specimens.

ID31, High-Energy Beamline for Buried Interface Structure and Materials Processing, is one of the new, long, microfocus, beamlines constructed during the ESRF Phase I upgrade program. The beamline also has a CdTe Pilatus detector, and offers a number of hard X-ray characterisation techniques including reflectivity, wide and small angle diffraction, imaging methods, and auxiliary techniques, coupled with versatility in choosing beam sizes, energy and energy bandwith.

Between them, these beamlines offer opportunities to study the crystal structures of materials via classic diffraction techniques, and to study the evolution of materials as they are heated or cooled, undergo chemical reaction, adsorb or desorb gasses, or generally are operated upon or processed under realistic operating conditions. Where appropriate, by tuning the photon energy to an element's absorption edge, anomalous scattering can be exploited to enhance contrast between elements close to each other in the Periodic Table. Defective, poorly-crystalline materials, glasses and liquids can be investigated structurally via the PDF technique, exploiting measurements to high Q values accessible via the hard energies available to yield a picture of short-range order and longer-range interatomic distances. Tomographic and other imaging techniques can yield detailed 3-d information of the grain-structure and phase distribution in polycrystalline and composite materials, yielding microstructural information on the length scales up to mm.

The talk will give an overview of some of the possibilities available at ESRF.

L-15 **Thursday, 07.09., 11^{30} – 12^{00}**

Solaris Synchrotron – from the start up to first experiments

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The Solaris synchrotron installed in Krakow represents a novel approach to the design of the third generation light sources. The 1.5 GeV storage ring consists on 12 integrated Double Bend Achromat (DBA) magnets designed in MAX-IV Laboratory in Sweden [1]. Integrating the DBA cell in one magnet block assures the alignment within tens of micrometres tolerances. Moreover, using strong focusing and multifunction magnets makes the storage ring lattice ultra compact reaching excellent beam parameters with the natural emittance of 5.98 nmrad [1]. The commissioning of Solaris storage ring started in May 2015 and required a big effort in machine parameters optimization [2, 3]. After 2 years of operation very good performance has been achieved. The optics was corrected close to the design values. Up to now over 400 Ah of the integrated current was accumulated in the storage ring and the average pressure with 250 mA of a stored current is $2.2 \cdot 10^{-9}$ mbar. The maximum stored current at the full energy is 400 mA with the total lifetime of 8 h. The lifetime of the beam is still increasing with the accumulated beam dose showing significant improvement since last year (Fig. 1) [4]. Apart from the vacuum conditioning, some minor adjustments are still needed in order to reduce the disparity between model and measured results what is the scope of current activities [5]. Moreover, during daily operation the main task is to maintain long-term stability of the circulating electron beam allowing for UARPES and PEEM/XAS beamlines commissioning. Within this presentation the overview of commissioning results and current Solaris facility status will be reported.

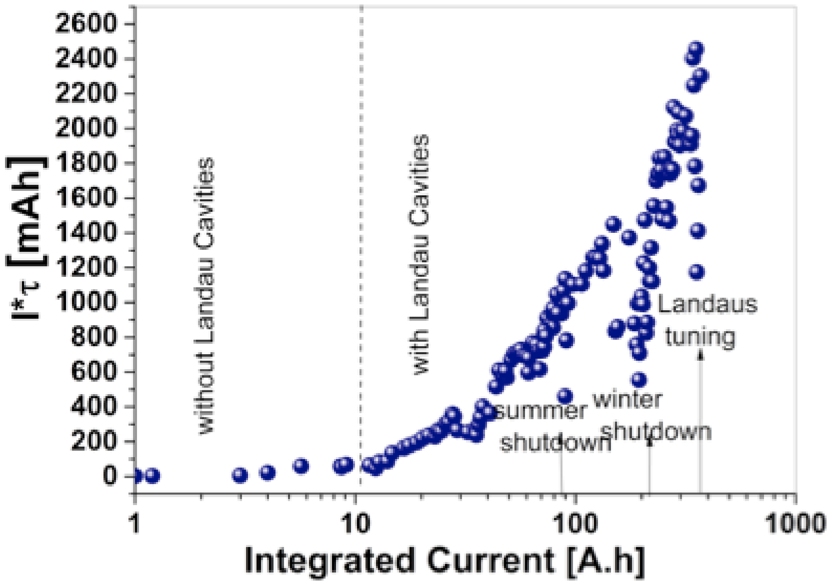

Figure 1. I*τ product vs. integrated current.

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[1] “MAXIV Detailed Design Report” *http://www.maxiv. lu.se/accelerators- beamlines/accelerators/ accelerator-documentation/max-iv-ddr/*

[2] A. I. Wawrzyniak et al.: “First Results of Solaris Synchrotron Commissioning” *Proc. of IBIC2015* **WEDLA01** (2015) 602.

[3] A. I. Wawrzyniak *et al.:* “Solaris a new class of low energy and high brightness light source” *Nuclear Inst. and Methods in Physics Research, B* (2017) in press; *https://doi.org/10.1016/j.nimb.2016.12.04.*

[4] A. Marendziak *et al.:* “Residual gas in the vacuum system of the Solaris 1.5 GeV electron storage ring” *Proc. Of IPAC2017* **WEPAB068** (2017) in press.

[5] A .I. Wawrzyniak, A. Kisiel *et al.:* “Performance of Solaris storage ring” *Proc. of IPAC2017* **WEOCA1** (2017) in press.

L-16 **Thursday, 07.09., $12^{00} – 12^{30}$**

Angle-resolved Photoelectron Spectroscopy at National Center for Synchrotron Radiation SOLARIS

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The research technique of Angle-Resolved Photo-electron Spectroscopy (ARPES) enables experimental determination of the allowed quantum states space for electrons, in solid state. The results provided by the technique are interpreted in general one-electron framework, however, at the second look many-body effects are revealed as well. Many recent scientific key results, concerning for example: high temperature superconductors, topological matter, graphene, have been obtained using ARPES. With reference to that the meaning of ARPES for advances in contemporary physics and technology is widely recognized. In SOLARIS an undulator based experimental line for the Angle-Resolved Photoelectron Spectroscopy has been constructed as one of the first. The line is called UARPES (after Ultra ARPES).

In this presentation the construction of the UARPES beamline as well as the available research opportunities will be presented and discussed. Also, there will be discussed the fundamentals of generation of synchrotron radiation beams in undulators and benefits of using such beams as an excitation for ARPES.

L-17 **Thursday, 07.09., $12^{30} – 13^{00}$**

Status and first results of the PEEM/XAS beamline commissioning process

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The PEEMXAS beamline has been optimized for the soft X-ray photn energy range (200-2000 eV) with the bending magnet as a synchrotron radiation source. The chosen optical design based on the plane grating monochromator working in the collimated light (cPGM) has been adjusted by the Optical Group from Elettra. The cPGM is equipped with two gratings to obtain energy resolution ($\Delta E/E$) in the order of $2.5\text{x}10^{-4}$ or better in the accessible energy range and available linear horizontal and elliptical polarization.

Within the framework between Jagiellonian University and Jerzy Haber Institute of Catalysis and Surface Chemistry PAS, the Photoemission Electron Microscope will be the main end station of the beamline. Exchangeable with microscope we use separate chamber for X-ray absorption spectroscopy measurements. It will be dedicated to experiments in the field of biology, chemistry, catalysis, material science and physics. Both stations are composed of several vacuum chambers including dedicated chamber for sample preparation and characterization under UHV conditions. The dimensions of the focused photon beam at the sample place are 100μm (H) x 50μm (V).

We summarize the commissioning phase of the front end components. The spatial stability of the source was characterized using the X-ray beam position monitors. Some small beam instabilities were discovered and preliminary feedback was implemented. This presentation reports on the PEEM/XAS beamline actual time schedule and the results of the first phase of the commissioning process.

Acknowledgements: Authors would like to thank A. Bianco, E. Busetto and I. Cudin from Synchrotron Elettra, Trieste for beamline optical design optimization and support during design period and also J. Raabe from Swiss Light Source at Paul Scherrer Institute for help in solving of many technical aspects.

L-18 **Thursday, 07.09., 13^{00} – 13^{30}**

Future beamlines at SOLARIS

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The plans of the development of Polish synchrotron SOLARIS in the incoming years are presented. Besides two existing beamlines, two next ones have been financed. One of them is PHELIX which will be based on radiation from the EPU type undulator in the energy range 50-1500 eV and with variable polarization. The collimated PGM monochromatization will be based on three gratings giving the resolving power better than 10^4 and flux density at the sample of 10^{11}photons/s/0.1BW. The techniques available at the endstation will be photoelectron spectroscopy in the angle integrated, angle resolved modes and in the spin resolved mode. Additionally x-ray absorption measurements in the TEY and TFY modes will be possible. Research opportunities available at PHELIX will be presented.

The XMCD beamline which is based on the former I1011 transferred from Maxlab. Their reinstallation at SOLARIS will require a necessary upgrade. The beamline is using radiation from the EPU undulator in the energy range 100-2000 eV. It will provide radiation for one of three endstations devoted to studies of materials with the use of x-ray magnetic dichroism.

The plans for the development of next beamlines will be also presented.

O-01 **Monday, 04.09., 10^{55} – 11^{15}**

A test linear accelerator for FEL development

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A concept of electron linac has been developed at NCBJ consisted of all-superconducting electron injector, Tesla-like accelerating section and plane, tunable gap undulator. The primary scientific case are the injector optimization, RF field and beam characterization while continues wave operation, dedicated for FEL development. THz-IR ranged electromagnetic radiation will be delivered to the experimental station.

O-02 **Monday, 04.09., 12^{45} – 13^{05}**

Quantum X-ray lasers pumped by XFEL radiation

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Success of the Linac Coherent Light Source (LCLS) proved that advent of the X-ray free electron lasers changed in some way the paradigm of the important research directions. Plasma X-ray lasers dominated unchallenged the field of short-wavelength generation until the FLASH facility began deliver the first photons. What is the relation between the both types of the short-wavelength sources? Is any chance for cohabitation? To answer these questions the output beam quality of both types of sources will be analysed in detail. The output parameters such as coherence and polarisation will be related to the mechanisms underlying the emission process. Finally, it will be shown the possible solution joining both system in a one where XFEL would be used as unprecedented pumping source initiating quantum excitation of the electronic system and forcing it to generate as a quantum X-ray laser conserving the best features of the pump and improving its biggest deficits, e.g. poor longitudinal coherence. The fundamental processes of such an interaction between hard X-rays and matter will be discussed in categories of the nonlinear spectroscopy, stimulated emission, saturation and medium kinetics. The first such a system has been realised at LCLS in 2011 using neon as the active medium and the result was reported in [1]. This inner-shell X-ray laser was realisation of the old proposal from 1967 [2], that has not be demonstrated in plasma in spite of major efforts. Further development of this pumping method will be surveyed and the potential research direction will be sketched. Here, solid targets are considered as the most promising while the hitherto attempts were focused on gases and solutions. A sketch of the proposed experiment is shown in Fig.1.

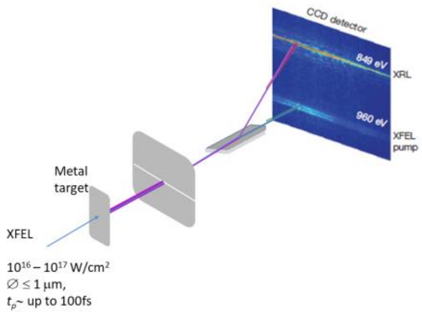

Figure 1. Arrangement of the quantum X-ray laser.

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[1] N. Rohringer, D. Ryan, R. A. London, M. Purvis, F. Albert, J. Dunn, J. D. Bozek, C. Bostedt, A. Graf, R. Hill, S. P. Hau-Riege, J. J. Rocca: *Nature* **481** (2012) 488.
[2] M. A. Duguay, G. P. Rentzepis: *Appl. Phys. Lett.* **10** (1967) 350.

O-03 **Monday, 04.09., 13^{05} – 13^{25}**

Micro- X-Ray fluorescence spectrometer with X-ray single bounce gold capillary optics for light element analysis

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In the last 20 years rapid development of X-ray optics was found application in micro X-ray fluorescence spectrometry (micro-XRF) and has become a powerful tool to determine the spatial distribution of major, minor and trace elements within a sample. Micro-X-ray fluorescence (micro-XRF) spectrometers for light element analysis ($6 \leq Z \leq 14$) using glass polycapillary optics are usually designed and applied to confocal geometry. The first capillary focuses the primary beam on the sample; the second restricts the field of view of the detector. In order to be able to analyze a wider range of elements especially with ($6 \leq Z \leq 14$), both sample and detector are operated under vacuum. Depth resolution varies between 100 µm at 1 keV fluorescence energy (Na-Kα) and 30 µm for 17.5 keV (Mo-Kα) [1,2]. In order to improve lateral and depth resolution, our group designed similar spectrometer (in cooperation with PREVAC) but instead of primary polycapillary optics we applied single bounce metallic capillaries optics, designed, manufactured. For single bounce capillaries the second capillary normally mounted in the front of detector is not needed. As a source, X-ray tube with microspot (40µm) was applied, similar as it was used in other spectrometer [1]. Our spectrometer was installed on December 2015 in our Laboratory.

Single bounce gold capillaries with elliptic internal shape have recently been redesigned and developed in our Laboratory. Surface roughness internal reflectivity layer was reduced up to 0.3 nm and slope error to ~ 0.05 mrad. Because capillaries are produced by electroforming method, X-ray reflectivity internal layer is not only limited to gold but other metals and multilayers are also possible. The spectrometer equipped with gold capillaries offers the possibility of elemental analysis with better lateral and depth resolution than is offered by glass polycapillaries at energies 9 keV (Cu, Kalpha) and 17.4 keV (Mo, K,alpha). To further extend analytical capabilities of single bounce metallic capillaries, we will present a design of a micro-XRF spectrometer using synchrotron radiation (SR). Capillaries with parabolic shape will be applied in order to focus SR and can be considered as a X-ray optics element for micro-XRF line of our Synchrotron SOLARIS . Furthermore, we will compare the capabilities and limitations of this spectrometer with others, that use laboratory and/or synchrotron sources.

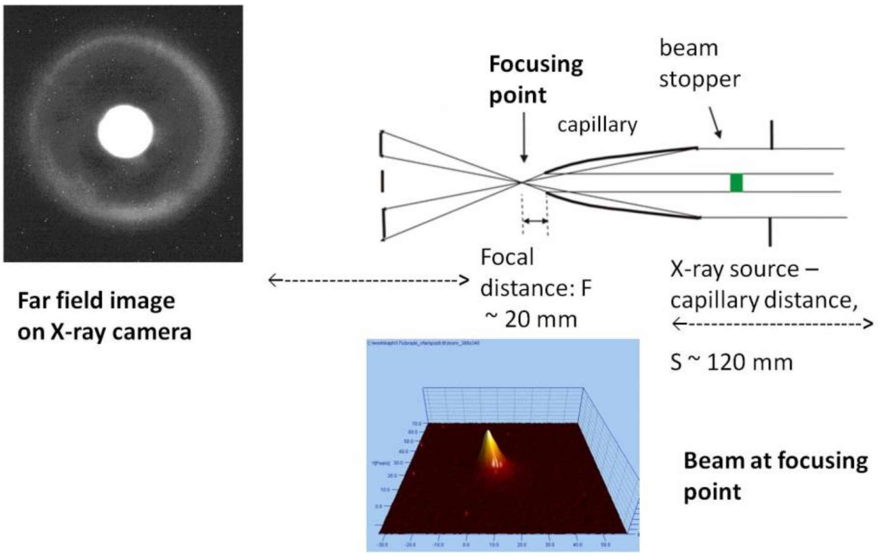

Figure 1. X-ray capillary optics setup.

Acknowledgements: This work was supported and co-funded by the European Union as part of the Operational Programme Development of Eastern Poland for 2007–2013, Priority I Innovative Economy, Measure I.3. Support for Innovations and The National Centre for Research and Development, Project no. TANGO1,267102/NCBR/2015.

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[1] S. Smolek, B.Pemmer, M. Folser, C. Streli, P. Wobrauschek: *Review of Scientific Instruments* **83** (2012) 083703.
[2] S. Smolek , T. Nakazawa, A. Tabe, K. Nakano, K. Tsuji, C. Streli , P. Wobrauschek: *X-ray spectrometry* **43** (2014) 93.

O-04 **Monday, 04.09., 15^{00} – 15^{20}**

Electronic state spectroscopy of small ether molecules in the gas phase

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We would like to present our findings on electronic structure of cyclic ethers: ethylene oxide, 1,3-dioxane and 1,3-dioxolane, which are important components of industrial production of solvents, stabilisers, plastics and larger organic molecules, like glycols, for household use. For example, ethylene oxide, the simplest one, can also be used as disinfectant in hospitals. Thus, throughout human actions they may play a role in the greenhouse effect.

We measured high resolution photoelectron spectra (Fig. 1) of the abovementioned cyclic ethers in order to derive their ionisation potentials, which in turn may be used to identify Rydberg states in VUV photoabsorption spectra that were also obtained (Fig. 2). With assistance of the state-of-the-art *ab initio* calculations we were also able to determine the valence transitions observed in the spectra. From the photoabsorption spectrum, the photolysis rates were determined in order to assess the probability of this mechanism being a key one for the removal of such molecules from the atmosphere. To date there is remarkably little data on the electronic states of these compounds.

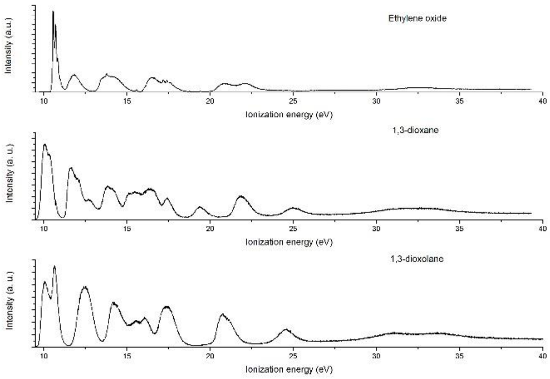

Figure 1. Photoelectron spectra of chosen ethers.

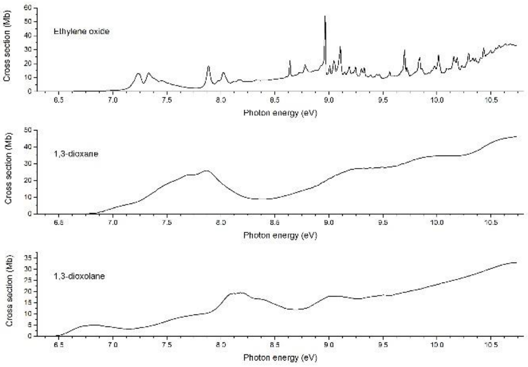

Figure 2. Photoabsorption spectra of chosen ethers.

Acknowledgements: The authors wish to acknowledge the beam time at the ASTRID synchrotron at Aarhus University, Denmark, supported by the European Union (EU) I3 programme ELISA, Grant Agreement No. 226716. Research described in this paper was performed at the Canadian Light Source, which is supported by the Canada Foundation for Innovation, Natural Sciences and Engineering Research Council of Canada, the University of Saskatchewan, the Government of Saskatchewan, Western Economic Diversification Canada, the National Research Council Canada, and the Canadian Institutes of Health Research.

O-05 **Monday, 04.09., 15^{20} – 15^{40}**

Inner-shell photoexcitation and fragmentation of isoxazole molecules at the K edges

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Synchrotron radiation being the most effective light source gives rise to significant developments in spectroscopic techniques, which probe the electronic structure and decomposition mechanisms of molecules. In particular the near edge x-ray absorption fine structure spectroscopy (NEXAFS) provides detailed information about presence of specific bonds and interactions in molecules.

In the present work we have used the soft x-ray excitation combined with techniques of pulsed field ionization and ion time-of-flight (TOF) spectrometry to investigate the gas-phase C1s, N1s and O1s excitation spectra of isoxazole molecules as well as a new class of mechanism of the photon-induced fragmentation, namely photoelectron recapture into the high-Rydberg (HR) states. The experiments were carried out at the Gas Phase Photoemission beamline at the Elettra synchrotron radiation facility exploiting the TOF mass spectrometer that was modified for pulsed field ionization measurements [1, 2]. This experimental set-up allows measurements of the total ion yield (TIY) and neutral HR fragments yield (HRY) without mass resolution. The same experimental setup can also be used for identification of the fragmentation products, by measuring the mass spectra of the HR fragments as well as the photoelectron-photoion coincidence maps (PEPICO). All of these spectra are necessary to elucidate the processes underlying the production of the neutral fragments being in the high-Rydberg orbitals.

The NEXAFS spectra of isoxazole were measured using the total ion yield method and were interpreted by means of time dependent density functional theory (TDDFT) calculations. Example patterns of experimental and theoretical (TDDFT SRC2-BLYP) C 1s NEXAFS spectra of isoxazole is shown in Figure 1. The most prominent transitions are indicated. Then, the production of neutral HR fragments after C1s, N1s and O1s inner-shell excitations/ionization and fragmentation of isoxazole was studied.

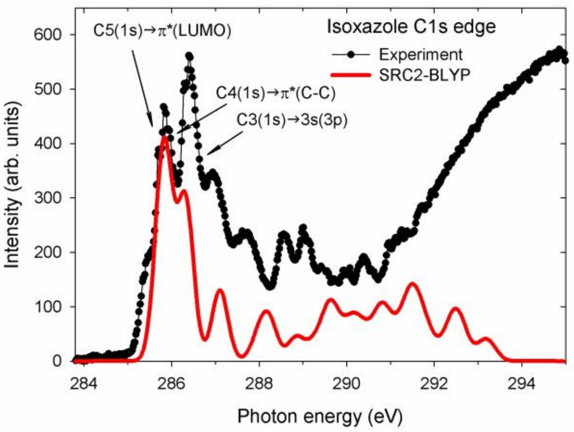

Figure 1. Experimental and theoretical C 1s NEXAFS spectra.

Figure 2 compares the total ion yield spectrum of isoxazole measured near the C1s edge without field ionization with the total yield of HR fragments (and energetic photons) obtained after applying field ionization.

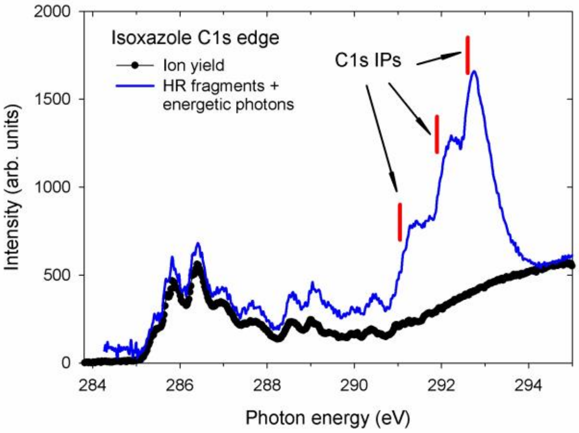

Figure 2. The TIY in comparison with the HRY at the C1s edge.

The HR spectrum resembles that of the TIY up to about 291 eV. However, near the C1s ionization thresholds a strong band arises, not observed in the TIY spectrum. The band is attributed to the production of neutral fragments in the HR states, that may be formed by recapture processes where photoelectrons are pushed back to be bound on the HR orbitals of the parent molecular ions after Auger decay [1, 2]. In order to identify particular neutral fragments in the HR states, a pulsed electric field was used to ionize them and resulting ions were mass-analyzed with an ion time-of-flight spectrometer.

Acknowledgements: This work was performed during the STSM visit of TJW to Elettra Sincrotrone, Trieste, and the financial support from the COST Action CM1204 (XLiC) is gratefully acknowledged.

[1] A. Kivimäki, *et al,*: *J. Chem. Phys.* **143** (2015) 114305.
[2] A. Kivimäki, *et al,*: *J. Phys. Chem. A* **120** (2016) 4360.

O-06 **Monday, 04.09., $15^{40} – 16^{00}$**

Photoionized plasmas induced by extreme ultraviolet or X-ray intense pulses

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Photoionized plasmas are common in Space where either X-ray or extreme ultraviolet (EUV) radiation is produced by different kinds of astrophysical objects and can propagate over long distances. Such plasmas are not encountered in normal conditions on Earth due to strong absorption of ionizing photons in atmosphere. Photoionized plasmas can be produced in laboratory conditions using intense EUV or X-ray radiation pulses. They can be utilized for scientific experiments, including laboratory astrophysics or astrochemistry, or can be employed for investigations concerning some technological processes.

In this work investigations of photoionized plasmas were performed using laser-produced plasma (LPP) EUV or soft X-ray (SXR) sources with various parameters. The sources were based on three different laser systems with pulse energies ranging from 0.8 J to 500J and pulse duration 0.2 ÷ 10 ns. Laser plasmas were produced by irradiation of double stream gas puff targets with Xe or Kr/Xe mixture as the working gas. In case of using the high power laser pulses (PALS, Prague) intense SXR pulses were produced. In case of using lasers of low energy, up to 10 J, emission in EUV range dominated the plasma radiation. The EUV radiation was focused using grazing incidence collectors based on multifoil, ellipsoidal or paraboloidal mirrors optimized for specific wavelength ranges. Photoionized plasmas were produced by the focused EUV radiation. Concerning the SXR radiation, gases to be ionized were injected and irradiated in the vicinity of the laser plasma or the radiation was focused onto the gas stream using the paraboloidal collector.

Gases to be irradiated, were injected into the interaction region, perpendicularly to an optical axis of the irradiation system, using an auxiliary gas puff valve. Photoionized plasmas were created in different gases either atomic (noble) or molecular. In all cases photon energies of the driving photons exceeded binding energies of outermost electrons. In case of the LPP EUV sources photon energies at spectral maximum were at the level of 100 eV. Energies of the SXR photons exceeded 1 keV. Taking into account that the highest ionization energy in case of a neutral gas is 24.6 eV (helium) photoionization events resulted in releasing of photoelectrons with energies sufficiently high for further ionization or excitation processes. It should be pointed out that energies of either EUV/SXR photons or photoelectrons were sufficiently high not only for ionization of atoms or molecules but also ions. This way photoionized plasmas containing multiple charged ions could be created.

Spectra in SXR/EUV range were measured using a grazing incidence, flat-field spectrograph equipped with a 450 lines/mm toroidal grating and a home made spectrograph based on free standing transmission grating 5000l/mm. The UV/VIS spectra were measured using an Echelle Spectra Analyzer ESA 4000. The spectra were composed of spectral lines corresponding to radiative transitions in atoms, molecules, atomic or molecular ions. For analysis of the EUV spectra numerical simulations were performed, using a collisional-radiative PrismSPECT code. Parameters of the photoionized plasmas were estimated by fitting the spectrum obtained from the simulations to the experimental one. For computer simulations of the molecular spectra measured in the UV/VIS range a LIFBASE code was employed. Apart from that, the electron temperatures were estimated by a Boltzmann plot method.

Acknowledgements: This work was supported by the National Science Centre, grant agreement no. UMO-2016/21/B/ST7/02225 and partially by European Union's Horizon 2020 Programme (LASERLAB-EUROPE) grant agreement no. 65414.

O-07 **Tuesday, 05.09., 9^{30} – 9^{50}**

Towards hybride systems - ARPES and STM/STS investigations of graphene, transition metal dichalcogenides and topological insulators

Iaroslav Lutsyk[1], Ewa Lacinska[2], Pawel Dabrowski[1],
Maciej Rogala[1], Natalia Olszowska[3],
Marek Kopciuszynski[4], Andrzej Wysmolek[2],
Mieczyslaw Jalochowski[4], Jacek Kolodziej[3],
Zbigniew Klusek[1]*

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Graphene is a material that has unique properties allowing for the movement of charge carriers at very high speeds. Moreover, spinlabeled charge carriers can travel in graphene with distances comparable to those encountered in superconductors. This makes graphene an interesting system for applications in spintronics. Unfortunately, the use of graphene in electronics and spintronics is limited due to the fact that this material does not have an energy gap. However, the combination of graphene with transition metal dichalcogenides (TMDC) and topological insulators can create a new class of materials called hybrid materials in which spin polarized charge carriers can be created and transported without scattering. This types of modern hybrid materials would help in the future to develop the next generation of computer systems.

We start from the basic physics of graphene, TMDCs, topological insulator and foundation of hybrid systems. In the central part of presentation we will show application of angle resolved photoemission spectroscopy (ARPES) with combination of scanning tunnelling microscopy and spectroscopy (STM/STS/CITS) techniques in studies of growth of graphene on SiC(0001) and Ge(001) substrates, charge density modulation in TaS_2 which is example of TMDC and electronic structure of topological insulator. We show ARPES results collected by standard laboratory source of light and preliminary results collected in UARPES beamline at SOLARIS facility. Especially, we focus on correlation of E(k) data obtained by ARPES with local density of states function LDOS(x,y,E) collected by STS/CITS. The obtained results will be discussed in the frame of DFT calculations performed using QUANTUM ESPRESSO code utilizing plane wave basis set and Projector Augmented Wave method. The representative set of data collected for TaS_2 is presented in Fig.1. They show (from left to right) 50 nm x 50 nm STM topography of TaS_2, LDOS profile measured by STS, spatial distribution of LDOS measured by CITS and ARPES data together with DFT calculation of band structure for TaS_2.

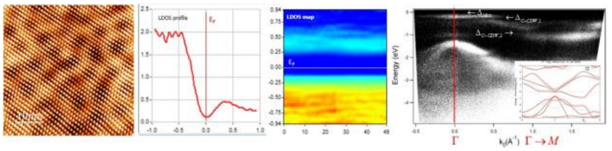

Figure 1. Representative data for TaS_2.

Acknowledgements: The work was financially supported by National Science Centre project: 2015/19/B/ST3/03142.

O-08 **Tuesday, 05.09., 9^{50} – 10^{10}**

Usefulness of photoelectron spectroscopy to study surfaces and interfaces: selected examples

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One of the main goals of materials science is to design materials with desired/required properties: mechanical, electrical, magnetic, optical, thermal and/or chemical. Besides simply having such properties, these materials need to be stable under conditions that they will normally encounter. Surfaces/interfaces play an important role in stability of the materials and, of course, affect the properties of underlying solid [1]. That is why surface/interface analysis with the ability to distinguish the findings from the ones from underlying solid, is not just one of the important studies, but is a necessity. Recent advancements on most of the frontiers of material science are noted in surface science as well. Refined instruments, detailed modelling, and deep and correct understanding of all processes have led to a situation where techniques, such as standard Photoelectron Spectroscopy as well as Resonant Photoelectron Spectroscopy, are successfully used on extremely complex structures.

This talk will present the results of X-ray Photoelectron Spectroscopy (XPS) and Resonant Photoelectron Spectroscopy (RPES) studies used to characterize surface/interface in two systems: Co/MgO with/without gold interlayer and ZnO:Yb, where both a laboratory spectrometer and synchrotron radiation facility were used.

Acknowledgements: This work was partially supported by the EAgLE international project (FP7-REGPOT-2013-1, Project No. 316014) and the international project co-financed by Polish Ministry of Science and Higher Education, Grant Agreement 2819/7.PR/2013/2.

O-09 **Tuesday, 05.09., $12^{00} – 12^{20}$**

Extended Abstract

CLD - atomic Column Length Distribution and Crystal Lattice Dynamics of supported gold catalysts. The key to understand their catalytic activity

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The question that our research aims to answer is the source of activity of heterogeneous catalysts based on nanocrystalline gold (Au). If appropriately synthesised, they exhibit particularly interesting chemical properties under milder reaction conditions than other comparable catalytic systems. In order to explain the extraordinary catalytic properties and to study the mechanism of how gold catalysts work, several techniques are employed, all of which were adopted for *in-situ*measurements:

1) NPD (Nanocrystalline Powder Diffraction),
a customised technique based on PXRD (Powder X-Ray Diffraction) coupled with MS (Mass Spectrometry) or both MS and XAS (X-Ray Absorption Spectroscopy),
2) EM (Electron Microscopy, particularly *in-situ* TEM – Transmission EM and ESEM – Environmental Scanning EM),
3) atomistic simulations.

We suggest that the experimentally observed catalytic properties of gold result from cyclic changes of the nanocrystals' surface structure, which occur due to interactions of the surface with adsorbing species. Examination of this process and precise description of the conditions, in which it happens, are crucial for fundamental understanding of the real source of catalytic activity of nanocrystalline gold.

It can be clearly seen after the analysis of the series of powder diffraction patterns, correlated with the on-line monitored reaction yield, that the crystal structures of both gold and the support (ceria, CeO_2) change dynamically with the varying reaction environment (see Fig. 1). Structure modifications are represented by the shift of reflections' positions and alteration of their shape. At first these phenomena are rather difficult to be interpreted properly. Here come the new interpretation methods developed along with the NPD technique. First, it is possible to fit the experimental data with a predicted pattern calculated via Debye summation formula [1] on the basis of an optimised atomic model of the nanocrystal. Next newly discovered option is to express the diffraction pattern changes in terms of evolving atomic columns' length distributions (CLD, [2]). We propose in [2] a complete method for CLD calculation based on a single reflection coming from a nanocrystalline strain-free metal. Its most valuable advantages are:

a) the assessment of the real background level with respect to a physical criterion, which is the positivity of the CLD,
b) the full procedure describing how to fit the peak profile with Voigt functions (see Fig. 2) and how to use them for calculation the CLD utilising the Warren-Averbach analysis method.

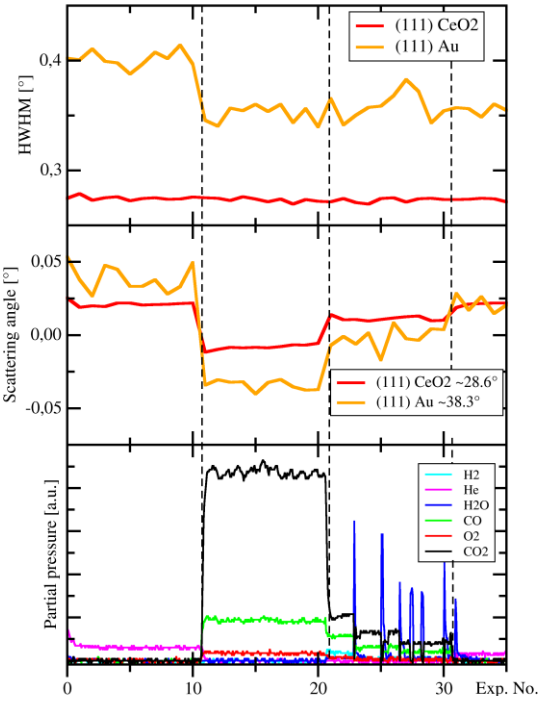

Figure 1. The set of graphs presenting the most recent results of investigation of the 10% Au/CeO[sub]$_2$[/sub] catalyst. The catalyst was exposed subsequently to helium, mixture of carbon monoxide and oxygen (reagents for stoichiometric CO oxidation reaction; volume ratio = 2 : 1), mixture of carbon monoxide, oxygen and hydrogen (reagents for PROX reaction, volume ratio = 2 : 1 : 4) and helium again (for reference purposes). All of the data are plotted as a function of measurement time normalised to the time required for one diffraction pattern acquisition. The upper graph presents the changes of Half Width at Half Maximum (HWHM) of the gold (111) and (220) diffraction peaks. The middle graph presents the change of the positions of selected diffraction peaks – (111) reflection of ceria, (111) and (220) reflections of gold. The bottom graph shows the results of the mass spectrometry analysis of the gas outlet stream leaving the reaction chamber.

Following the evolution of CLD allows to track the anisotropic shape changes of the crystals while taking into consideration the crystal size distribution (see Fig. 3). This is a priceless structural information about the behaviour of the catalyst under reaction conditions.

Furthermore, the NPD technique is capable of discovering the formation of new crystal phases and structure reconstruction that the gold catalyst may undergo in *operando* conditions (see Fig. 4). Such an important evidence helps to resolve the possible active or inactive states of the gold catalyst.

Although PXRD measurements provide plentiful information about the studied system, it is always an averaged view over the whole sample, all crystals and atoms building them. As it is the surface which is the most interesting part of the active gold catalyst, the additional ability to distinguish the surface from the interior of the gold crystals is considered to be vital. The incorporation of XAS arises a new opportunity to differentiate between the atoms located inside the crystal's structure and those, that take part in interactions of the crystal’s surface with the environment.

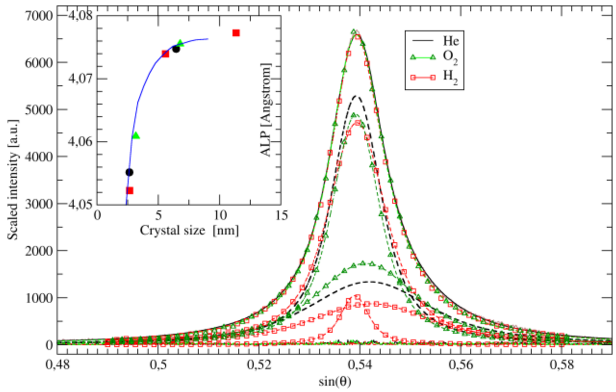

Figure 2. 220 diffraction peaks for the 20%Au/C catalyst exposed to the atmosphere of helium, oxygen and hydrogen fitted by 2 (He, O_2) or 3 (H_2) Voigt functions (dashed lines). Insert: Apparent Lattice Parameter [3] calculated from the Voigt profiles as function of mean crystals size according to Scherrer formula.

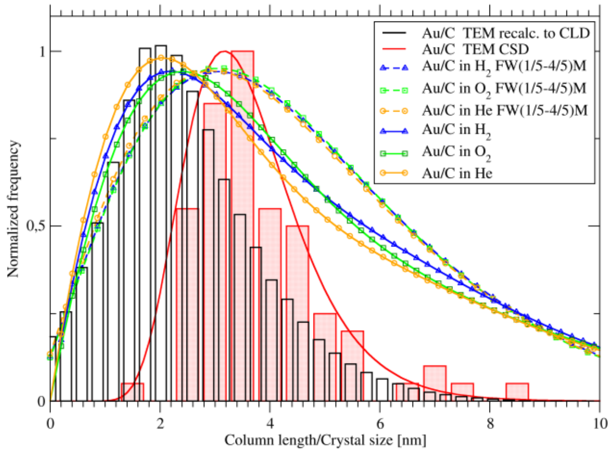

Figure 3. The Column Length Distribution (CLD) calculated with our new method [2] in case of the 20% Au/C catalyst exposed to helium, hydrogen and oxygen atmosphere (solid lines), compared with the Pielaszek method (FW(1/5-4/5)M, dashed lines, [4]) and TEM crystals size distribution (CSD) analysis results recalculated to CLD (red and black solid lines. For details, please refer to [2].

The atoms lying closest to the crystal’s surface change dynamically their energy and electron state according to adsorption and desorption of reagents and reaction product. The differences of states are then reflected in the XAS spectrum. In addition, the smaller are the gold crystals, the bigger is the surface to volume ratio and the more visible are the differences between the subsequent XAS spectra. Thus, XAS coupled with PXRD and MS serves its powerful capabilities for thorough investigation of heterogeneous gold catalysts offering simultaneously new complementary structural data under *operando* reaction conditions.

Combining the results obtained with PXRD, MS and XAS it is possible to develop the catalyst model and to deduce the way how the catalyst works. With the aid of EM the model can be verified through *in-situ* structure studies with atomic resolution.

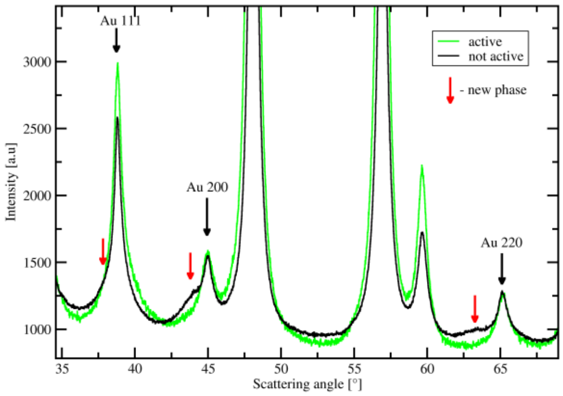

Figure 4. Diffraction patterns collected in the atmosphere of helium and after the PROX reaction showing new diffraction peaks corresponding to formation of a possibly new crystallographic phase during the PROX reaction which slowly leads towards deactivation of the catalyst.

The structure evolution is recorded in a series of high resolution images which show the projection of the crystal lattice along a chosen crystallographic direction.

It becomes possible to see directly the distortion of the catalyst’s crystals’ lattices and the ALP (Apparent Lattice Parameter, [3]) distribution throughout the crystals’ volume. Such a deep insight into the catalyst structure enable even the assessment of the thermodynamics of the reaction taking place on the gold surface, which was not possible before.

To conclude, the research introduced here combines uniquely the in-laboratory studies with synchrotron measurements and electromicroscopy investigation creating possibly the most complete image of the working catalyst explaining its crucial properties on fundamental level.

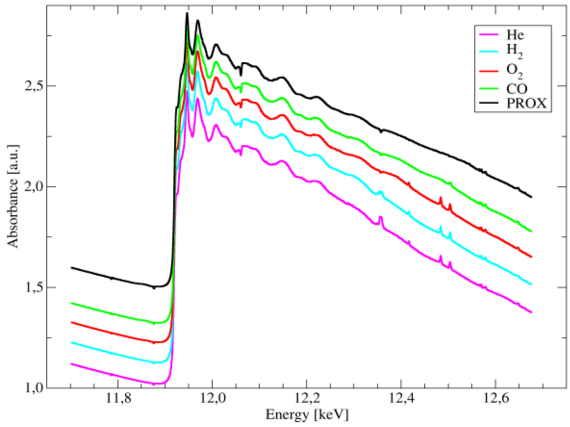

Figure 5. Raw XAS spectra acquired for the 10%Au/CeO_2 catalyst in different gaseous atmospheres.

Acknowledgements: This work was supported by National Science Centre of Poland, research grant no. 2014/13/B/ST4/04619.

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0-10 **Wednesday, 06.09., 9^{30} – 9^{50}**

Determination of oxygen vacancy limit in Mn substituted YSZ ceramics

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Yttria Stabilized Zirconia (YSZ) is commonly used as electrolyte in Solid Oxide Fuel Cells (SOFCs). During operation SOFC undergoes gradual degradation due to destructive interactions at interfaces and surfaces of the materials building the cell [1, 2]. Among the possible ways to ameliorate cell operation is intentional mixing of electrodes and electrolyte materials in order to improve theirs compatibility and stability [3]. In particular the application of Mixed Ionic-Electronic Conductors (MIECs) as a cathode material [4] or as thin layer on the surface of the electrolyte [5]. Therefore manganese doping into cubic YSZ was proposed for modification of typical SOFC electrolyte working in contact with $LaMnO_3$ cathode [1].

Important parameter that influences ionic conductivity and thus cell performance is the number of oxygen vacancies generated by aliovalent dopants in ZrO_2. Yttrium (3+) substituting for zirconium (4+) generates oxygen vacancies necessary to stabilize ZrO_2 in cubic structure. Manganese introduces additional vacancies, but as a dopant it can adopt different oxidation states and thus the structural and chemical changes it introduces with respect to doped material are difficult to predict. Determination of the oxidation state of Mn ions allowed to estimate the amount of oxygen vacancies in YSZ ceramics generated by dopants.

The series of $Mn_x(Y_{0.148}Zr_{0.852})_{1-x}O_{2-\delta}$ ceramics was systematically studied by means of X-ray Absorption and Emission Spectroscopy and DC magnetic susceptibility. XAS and XES results show changes in manganese oxidation state and a gradual evolution of the local atomic environment around Mn ions upon increasing dopants content, which is due to structural relaxation caused by growing amount of oxygen vacancies.

Acknowledgements: Access to ESRF was supported by special project ESRF/73/2006 from the Polish Ministry of Science and High Education. JS and MS acknowledge support from the National Science Centre of Poland (2014/14/E/ST3/00026).

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0-11 **Wednesday, 06.09., 9^{50} – 10^{10}**

Determining the structure of novel bioactive Cu(II)-thiourea complexes by combined XAFS spectroscopy, laboratory techniques and DFT calculations

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Three new complexes of Cu(II) with ligands, consisting of thiourea system attached to polycyclic imide and Br substituted phenyl moieties, were obtained from the direct synthesis in the powder form. One of these coordination compounds was found to exhibit high antibacterial activity against *Staphylococcus* strains. As the attempts to crystallize studied complexes were unsuccessful, their structures were determined with spectroscopic techniques, notably X-ray absorption fine structure (XAFS) spectroscopy, combined with the density functional theory (DFT) computations.

Thiourea derivatives used in this work may act as multidentate *S*, *N*, *O*-ligands, therefore predicting the structure of new complexes without crystal data was not a trivial task. The chemical composition of studied compounds was established from combustion elemental analysis, followed by laboratory spectroscopic (infrared and UV-Vis) measurements. The electron paramagnetic resonance (EPR) confirmed the presence of (nearly) non-interacting Cu(II) centers in the samples. XAFS measurements at Cu K edge were performed in Elettra synchrotron (Trieste, Italy), in order to refine the coordination sphere of central ion.

The final structure of complexes were established upon feedback between XAFS data and DFT modeling. The series of molecular models, consistent with sample stoichiometry and preliminary spectroscopic data, were optimized at DFT level and for these structures the fitting of XAFS spectra was performed. The model corresponding both to the best match to XAFS data and the lowest energy in DFT calculation is the structure with peculiar coordination pattern, where Cu(II) ion is a member of 2 four-atoms rings, formed upon the chelation via S and N atoms from two ligand molecules. In two cases XAFS detected the presence of another Cu and S atoms in the second coordination shell, implying the dimerization of basal mononuclear complexes. DFT calculations confirmed the lack of coupling between paramagnetic centers in such dimers, reconciling EPR and XAFS results.

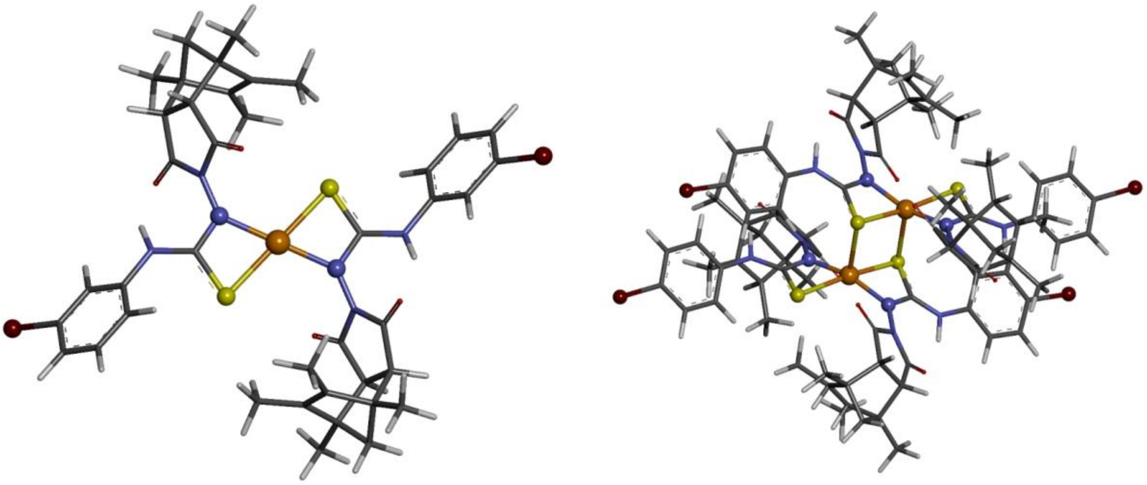

Figure 1. The structures of Cu(II)-thiourea complexes.

Acknowledgements: This work was partially supported by (1) the EAgLE international project (FP7-REGPOT-2013-1, Project No. 316014) and the international project co-financed by Polish Ministry of Science and Higher Education, Grant Agreement 2819/7.PR/2013/2, (2) PL-Grid Infrastructure (ACK Cyfronet and WCSS computational facilities) and (3) the Medical University of Warsaw and carried out with the use of CePT infrastructure financed by the European Union - the European Regional Development Fund within the Operational Programme Innovative Economy for 2007-2013.

0-12 **Wednesday, 06.09., 11^{00} – 11^{20}**

Specification of gene carriers based on ammonium gemini surfactants and siRNA enhancing DMPK gene in type 1 myotonic dystrophy (DM1)

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The main research subject that we have studied in a few last years, is the construction of non-invasive systems for transferring short oligomers of nucleic acids into the interior of cells, which would support successful gene therapy [1-4]. In particular, several groups of dimeric surfactant molecules have the desired ability to form highly organized and stable supramolecular structures with nucleic acids [5-7]. These surfactants, selected for therapeutic purposes, should be first carefully characterized, therefore they have been subjected to detailed analysis including structural and spectroscopic studies, analysis of their ability to self-organize and bind nucleic acids and the study of their effects on live cells. The conformation of nucleic acid in complexes formed on the basis of selected quaternary ammonium salt derivatives [8] and a specific 21-mer siRNA [9], was studied by circular dichroism (CD) and small angle scattering of synchrotron radiation (SR-SAXS). On the basis of agarose gel electrophoresis tests, we were able to determine the concentration of components required to form stable lipoplexes. Moreover, we determined non-toxic ranges of surfactants concentrations for model cell lines – one of the most important parameter in the target application these systems as gene carries. In the presentation we would like to show these results in relation to the studies already carried out on a similar group of amphiphilic compounds and complementary dsDNA oligomers.

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0-13 **Wednesday, 06.09., 11^{20} – 11^{40}**

Molecular structure investigation of coumarin complexes with Cu ions

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In the presented study determination of the binding mechanism between metal ion and organic ligand in two copper complexes with coumarin derivatives is shown. Coumarin is known for its wide range of biological activity (e.g. anti-inflammatory, antibacterial or cytotoxic [1]) and therefore it can be used as a scaffolding in the design of synthetic compounds that exhibit extensive pharmacological activity.

Both presented complexes exhibit selective activity against gram-positive bacteria. Unfortunately, obtaining these compounds in a crystalline form did not succeed. Therefore, to determine the geometry of complexes X-ray Absorption Spectroscopy (XAS) technique was applied. This method gives information about the local structure around the specific element and is ideal to study compounds regardless of their crystal form or state [2–3].

Measurements were performed at Cu K-edge (8979 eV) at XAFS beamline of the Elettra storage ring (Trieste, Italy). The XAS spectra were collected in transmission mode for powdered samples. Reference oxides were also measured. To gather structural information about copper complexes, both near edge structure (XANES) and extended fine structure (EXAFS) have been analyzed. Obtained information have been used to construct model which have been further analyzed to describe molecular structure of the investigated compounds. Additionally, DFT calculations and XANES simulations have been performed.

Described structural studies on the coumarin copper complexes provided detailed information about coordination geometry of copper cations in studied compounds.

Acknowledgements: Experimental research was funded from the Polish National Science Centre (Grant No. UMO-2012/07/D/ST5/02251). This research was supported by PL-Grid Infrastructure.

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0-14 **Wednesday, 06.09., 11^{40} – 12^{00}**

X-ray spectroscopy for analysis of metal anti-cancer complexes and their interaction with biomolecules

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The accidental discovery of the anticancer properties of cisplatin and its clinical introduction in the 1970s paved the way for the use of platinum based metallodrugs in chemotherapy. Second-generation analogues (e.g. carboplatin) were discovered shortly after. However, the clinical introduction of new anticancer metallodrugs has slowed down dramatically, especially considering the number of new drugs synthesized each year. Probably the most critical factor for this slow progress is the inability to elucidate in a timely manner how metallodrugs induce tumour death, precluding the rational development of new derivatives with enhanced anticancer capabilities. Most chemotherapeutic agents exert their antitumor effect by damaging DNA and its replication machinery. Therefore, the correlation between the covalent bonding to DNA and the cytotoxicity of the metal complex remains a central step in the search for new anticancer drugs.

Herein, we report a strategy to follow the chemical structure and coordination of platinum-based antitumor drugs by DNA under physiological conditions, namely by means of in situ resonant X-ray emission spectroscopy (RXES). RXES is an atom specific photon-in photon-out scattering technique which avoids the tedious steps of extraction and crystallization required by conventional X-ray techniques.

The spectroscopic method proposed by us was successfully used to validate the mechanism of action of cisplatin [1, 2] as well as elucidate the DNA binding of Pt103 compound that exhibits cytotoxic activity [3]. Moreover, we showed that RXES can be used to unveil the electronic structure of metallodrugs with high resolution and sensitivity and to disentangle differences in the electronic structure of the metal center induced by a secondary ligand stereochemistry [2, 4, 5].

Acknowledgements: J. Cz.-M. acknowledges National Science Centre, Poland (NCN) for support under grant no. 2016/21/D/ST4/00378.

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0-15 **Wednesday, 06.09., 15^{00} – 15^{20}**

Application of molecular dynamics simulations to interpret X-ray absorption spectra

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The effectiveness of classical molecular dynamics (MD) simulations for the interpretation of x-ray absorption fine structure (XAFS) of thermally activated decomposition of diluted magnetic semiconductors (DMS), namely, (Ga,Mn)As after medium temperature post growth annealing was tested. To determine the local atomic structure around Mn atoms XAFS spectra at Mn K-edge were gathered at about 90 K at BL22 beamline, ALBA synchrotron facility (Spain). The annealed samples show reorganization of the near edge electronic structure and dramatic decrease of the modulus of Fourier transforms amplitude, |FT(R)|, with annealing temperature increase. This decrease can be modeled either via (i) an increase of the Debye-Waller factor and/or (ii) a decrease of neighboring atoms number around Mn (which is a result of structural transformation caused by Mn atoms migration in GaAs matrix before formation of Mn-rich inclusions in GaAs matrix). The latter can take place only when As/Ga vacancies are considered as well. Taking this into account, various models with vacancies, as well as interstitial and substitutional point defects (Mn_{Ga}, Mn_i) were studied using MD simulations to produce theoretical EXAFS signals that were then directly compared to the experimental ones. Validation of the theoretical results by comparing to experiment allows us to derive previously unknown details of local structure around Mn in GaAs matrix after annealing treatment. This study demonstrates that MD simulations can accurately depict complex experimental systems in which we have control over high-level disorder, and shows the advantages of using a combined experimental/theoretical approach over standard EXAFS fitting methodologies for determining the structural parameters of such systems.

Acknowledgements: This work was partially supported by the EAgLE international project (FP7-REGPOT-2013-1, Project No. 316014) and the international project co-financed by Polish Ministry of Science and Higher Education, Grant Agreement 2819/7.PR/2013/2.

0-16 **Wednesday, 06.09., 15^{20} – 15^{40}**

Monte Carlo simulations of multiple scattering in Compton spectroscopy

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MUSCAT is a new Monte Carlo program for multiple scattering simulations of polarized high-energy X-rays for Compton experiments [1]. The code was developed to follow the restrictions of real experimental geometries (Fig. 1). The new simulation algorithm uses not only well known photon splitting and interaction forcing methods but it was also upgraded with the new propagation separation method and highly vectorized. The code has been verified by comparison with the previous experimental and simulation results by the ESRF group [2] and new restricted geometry experiments carried out at SPring-8 (Fig. 2). MUSCAT may also be useful in other research like Compton imaging or reflection XAFS.

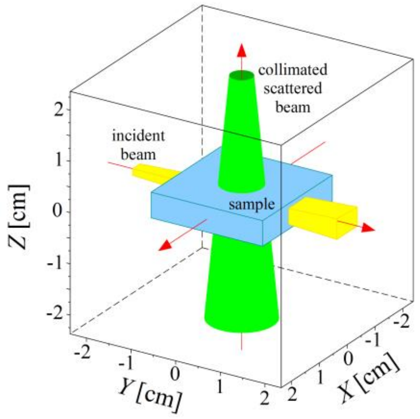

Figure 1. Sample geometry realised in the MUSCAT program.

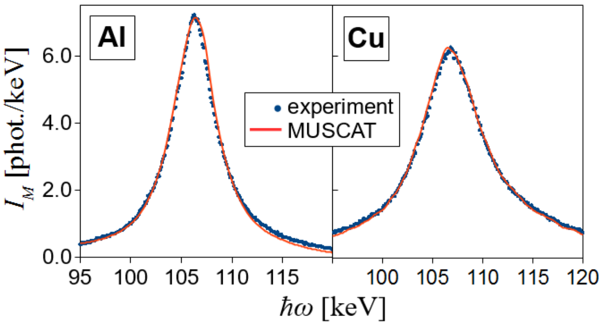

Figure 2. Experimental verification of MUSCAT program.

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[2] P. Fajardo, V. Honkimaki, T. Buslaps, P. Suortti: *Nucl. Instr. and Meth. B* **134** (1998) 337.

O-17 **Thursday, 07.09., 10^{30} – 11^{00}**

How to prepare and submit project to ESRF

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38000 Grenoble, France

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O-18 **Thursday, 07.09., 13^{30} – 13^{50}**

SOLARIS user office

Alicja Górkiewicz [1]*

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P-01 **Monday, 04.09., 16^{30} – 19^{00}**

FDTD simulations for determining optical properties of gold nanoparticles

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Arrays o spherical gold nanoparticles are a good candidates to be used as a biosensors (e.g. for a glucose), by studying their spectral response in different conditions. There are many ways to produce these arrays [1,2], and their optical properties are depended on many factors (e.g. size and distribution, substrate used, the light source).

In this wrk the Finite Difference Time Domain (FDTD) method is applied to study the optical properties of arrays of gold nanoparticles on a different substrates (ITO, glass) and of a different sizes and distributions. FDTD is a widely used numerical method, based on the Yee's grid, and is useful for solving the time-dependent Maxwell's equations. It's relatively fast (compared to the FEDT – Finite Elements method), but highly memory-consuming.

Calculated electromagnetic near-field distributions, intensities (see example on Fig.1) and plasmonic decay time are presented for a different distributions of the nanoparticles on the selected substrates (regular and random) as well as for a different light sources and wavelengths. In particular, strong enhancement of the electromagnetic field due to the plasmonic effect is shown. The influence of the FDTD simulation numerical parameters (e.g. grid size) is also discussed in details.

P-02 **Monday, 04.09., 16^{30} – 19^{00}**

Continuum contributions to the atomic electric dipole moments (EDM) of Xenon

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The multiconfiguration Dirac-Hartree-Fock (MCDHF) method has been employed to calculate the atomic electric dipole moments (EDM) of ^{119}Xe. EDM arising from (P;T)-odd e-N tensor-pseudotensor and pseudoscalar-scalar interactions, nuclear Schiff moment, interaction of electron electric dipole moment with nuclear magnetic moments, and atomic electric dipole matrix elements, was calculated with relativistic atomic structure package GRASP2K [1]. To estimate values of EDM for ^{119}Xe it is important to analyze the influence of continuum states. Wave functions of continuum states was computed with program COWF, then the EDM contribution was calculated in frames of the EDM B and EDM C codes [2], see Fig. 1.

The continuum orbitals are solutions of the Dirac–Fock equations. These equations are solved by the method of outward integration. The continuum wave function were normalized “per unit energy”.

The results show small contribution of continuum state electron o the final EDM value. Moreover, while increasing the set of the active orbitals, contribution from the continuum states decrease.

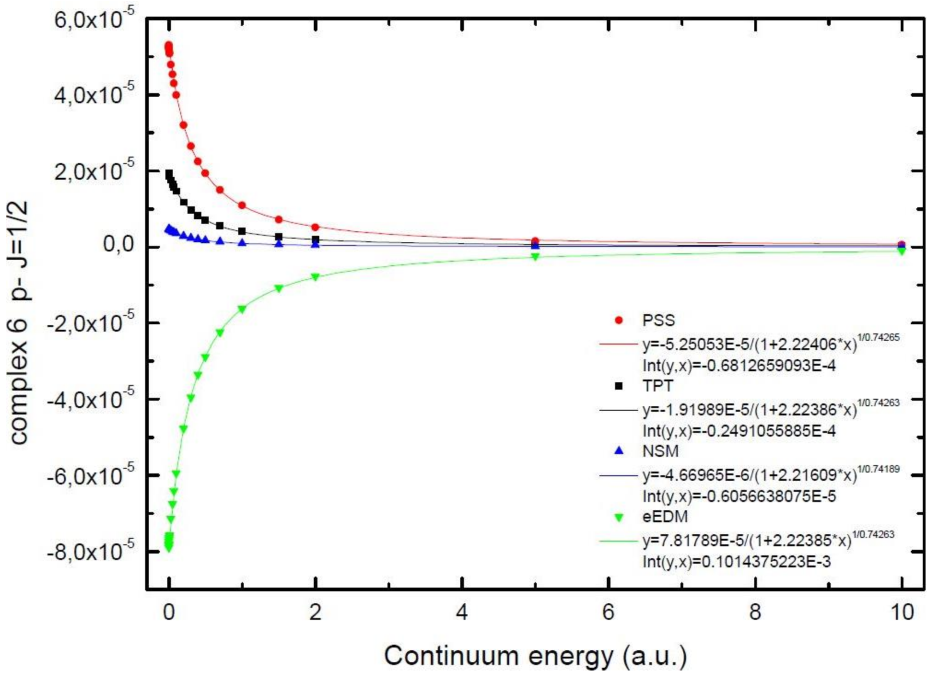

Figure 1. EDM contributions for different interactions.

Acknowledgements: Calculations were carried out at the Academic Computer Centre in Gdańsk.

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[1] P. Jonsson, G. Gaigalas, J. Bieroń, C. Froese Fischer, I. Grant: *Comput. Phys. Commun.* **184** (2013) 2197.
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P-03 **Monday, 04.09., $16^{30} – 19^{00}$**

Photoelectron and threshold photoelectron spectroscopy of pyridine

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Pyridine molecule (Fig. 1) was chosen as the subject of this study. This molecule is often used as a precursor to agrochemicals (bacteri- and herbicides) and medicines (sulfapyridine or tripelennamine) [1] and also utilized as a solvent or chemical reagent [2]. Many chemicals contain pyridine ring structure, like B-group vitamins or nicotine [3]. Investigations of this molecule are thus not only important due to its industrial or biological implications but are also valid for astrochemistry, since it has been shown that B-group vitamins can be found on the surface of meteorites [4].

In our work [5] we revisited on the subject of photoelectron spectroscopy investigations of the pyridine molecule. The photoelectron spectra of this molecule were measured at the VLS-PGM beamline at the Canadian Light Source facility in Saskatoon, Canada, using Double Toroidal Coincidence Spectrometer. Using such a high resolution photoelectron spectrometer, it was possible not only to resolve the inner and outer valence ionization energies (Fig. 2, top), but also, throughout the threshold electron measurements (Fig. 2, bottom), confirm the vibronic structure associated with most of the bands in the spectrum. This vibronic structure associated with several states was assigned mainly to be due to C–C stretches and ring bends. Additionally, a possible Rydberg state, converging to $7b_2$ state, was ascribed.

The data shown here are in an excellent agreement with previous results and brings some new insights into the electronic structure of pyridine molecule.

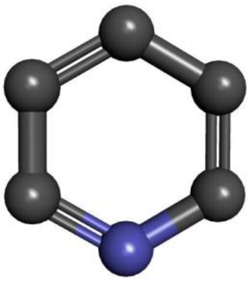

Figure 1. Pyridine molecule.

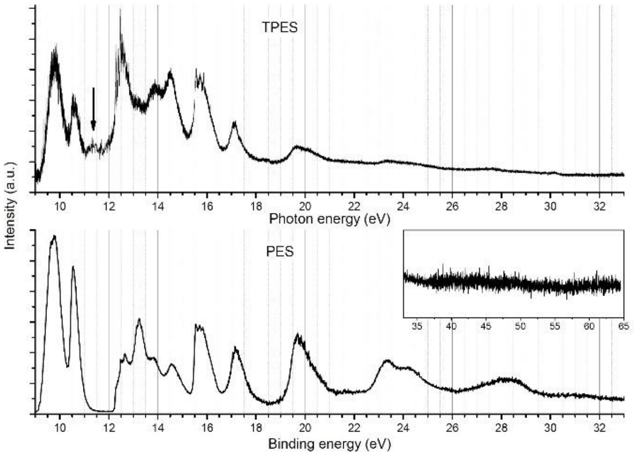

Figure 2. PES and TPES spectrum of pyridine.

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[1] M. Winston: *Arch. Dermatol.* **87** (1963) 489.

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P-04 **Monday, 04.09., $16^{30} – 19^{00}$**

Application of hard X-ray total scattering and Pair Distribution Function for characterization of amorphous Si-ferrihydrites

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Metastable non-crystalline two-line ferrihydrite $Fe_5HO_8 \cdot 4H_2O$ is the (oxy)hydroxide mineral with astonishing properties set by its highly defective structure. These properties are strongly affected by even small amounts of impurities (e.g. Si, C, P, As, S or Al), with Si being probably the most environmentally important. The effect of Si content has received particular attention recently because it hampers the thermal conversion of ferrihydrite into hematite α-Fe_2O_3, resulting in formation of other polymorphs: nanomaghemite γ-Fe_2O_3, luogufengite ε-Fe_2O_3 and β-Fe_2O_3 [1]. These amorphous iron(III) oxide nanoparticles take up a special place in nanomaterials science and advanced applications due to their intrinsic (i.e. stoichiometry, size, morphology etc.), magnetic, optical, and sorption properties [2]. Thermal phase transition of iron(III) oxide polymorphs provide an interesting systems for development of models to explain the formation of new nanomaterials. The transformation of Si-ferrihydrite into hematite via γ–ε or γ–ε–β pathway depends on the initial Si/Fe ratio (Fig. 1).

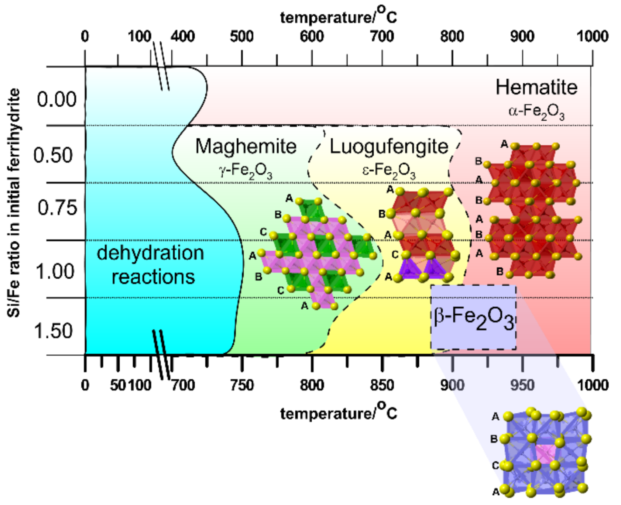

Figure 1. Ranges of stability temperatures for iron oxide.

Formation of rare epsilon and beta iron (III) oxide polymorphs from high-Si ferrihydrites can be explained by the formation of amorphous SiO_2 during annealing, which subsequently acts as anti-sintering agent stabilizing maghemite precursor against its direct thermal conversion to hematite [1]. Moreover, silicate exhibit negative or low thermal expansion in elevated temperature [3]. Such behavior may have an influence on distortions in structures of Si-doped iron(III) oxides, thus on the properties of products of their conversion.

Here we report the results of a detailed structural investigation using synchrotron-based pair distribution function analysis (PDF) and high-resolution X-ray diffraction (HR-XRD) on a series of Si-bearing synthetic analogues of ferrihydrite and products of their thermal transformation. Silicon content representing a range of Si/Fe a.f.u. ratio between 0.0 (pure phase) and 1.5 (doped phases) was used which is relevant to geological environments. Ferrihydrites were synthesized by precipitation from aqueous solutions of $Fe_2(SO_4)_3$ with NaOH in the presence of Na_2SiO_3 at pH 8.2. The products were characterized using powder XRD, X-ray scattering and Pair Distribution Function analysis, electron microscopy SEM/EDS, and differential thermal analysis (DTA and TG with QMS, from room temperature to 1000°C). The ferrihydrites were also heated to various temperatures selected based on the analysis of thermograms, and the intermittent products of transformation were identified and analyzed separately. The PDF and HR-XRD provide local structural information and allow for better understanding of the atomic-scale structure of poorly crystalline, disordered and nano-sized minerals. It allows also to establish a measure of particle size and crystallinity (Fig. 2).

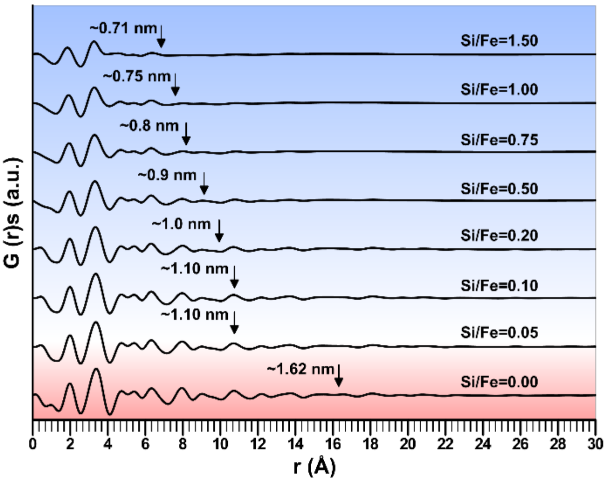

Figure 2. PDF [G(r) functions] of Si-ferrihydrite samples.

PDF analysis reveals systematic variation of the properties with increasing Si content in ferrihydrite: crystallite size decreases and the unit cell parameter c decreases while the unit cell parameter a increases. The analysis of hematite as a product of thermal transformation of Si-ferrihydrite indicates that Si is not present in the hematite structure. It crystallizes separately in the form of cristobalite.

Acknowledgements: This project is financed by the Polish National Science Centre under the research project awarded by the decision no. 2015/19/N/ST10/01516.

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P-05 **Monday, 04.09., 16^{30} – 19^{00}**

Extended Abstract

Electronic structure of carbon nanotubes decorated by platinum nanoparticles

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The discovery of carbon nanotubes in 1991 led to start a series of intensive studies into this new form of carbon, confirming their unique mechanical, electrical, thermal and optical properties [1, 2]. The chemical functionalisation of carbon nanotubes enables to develop completely new composite materials combining the unique properties of nanotubes and other materials, where it becomes possible to control their electrical, mechanical, thermal and optical properties [3, 4]. Deposition of nanoparticles of noble metals such as Pd, Pt, Rh, Au onto a surface of carbon nanotubes may contribute to a substantially higher density of carriers of free loads, hence to nanotubes enhanced thermal and electrical conductivity.

A one of a practical application of the so developed nanotubes-nanoparticles type materials are sensors of selected chemical substances, including H_2, CH_4 and NO_2 [5, 6]. The key advantages of sensors containing an active material in the form of a CNT-Pt composite are high chemical and thermal resistance, no requirement to work at an elevated temperature, as in a majority of optional solutions, operating sensitivity, fast reaction and selectivity.

In our study we presented the results of electronic structure of CNT-Pt type nanocomposite materials with a varying mass fraction of platinum nanoparticles.

Multiwalled carbon nanotubes with the length of 100-200 µm and diameter of 10-20 nm fabricated with the Chemical Vapour Deposition (CVD) technique were employed for investigations aimed at recognising the electron properties of the fabricated nanocomposite materials. 8% chloroplatinic acid H_2PtCl_6 supplied by Sigma Aldrich was used for synthesising the platinum nanoparticles.

Three sets of specimens containing, respectively, 5, 10 and 20% of platinum nanoparticles deposited on the surface of carbon nanotubes were prepared for spectroscopic studies. CNT-Pt-type nanocomposites were prepared by the preliminary treatment of the surface of carbon nanotubes with function groups (-COOH, -COH, =CO) through their covalent functionalisation in a mixture of acids. Platinum nanoparticles were synthesised by way of chemical reduction in the second phase of the process, and then they were deposited onto the surface of nanotubes.

The electronic structure of unmodified carbon nanotubes CNT and CNT-Pt-type nanocomposites were measured by X-ray Photoelectron Spectroscopy (XPS) and ultraviolet photoemission spectroscopy (UPS) methods. The C1s core level and the valence band measurements were performed on the monochromatic Al Kα=1486.6 eV excitation energy and a He lamp (HeII) with 40.8 eV excitation energy, respectively, using the PHI 5700 Physical Electronics spectrometer. In order to comparison of the density of states near Fermi level, the HeII valence band of a platinum foil and a graphite were recorded.

In figure 1 the transmission electron microscopy (TEM) photographs for three sets of specimens containing, respectively, 5, 10 and 20% of platinum nanoparticles deposited on the surface of carbon nanotubes were presented [7].

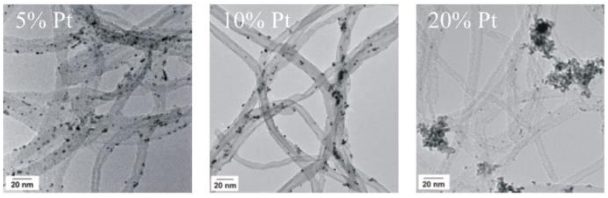

Figure 1. TEM photographs of CNT-Pt nanocomposites [7].

In case of a nominal deposition of 5% and 10% nanoparticles are rather homogeneously distributed, however for a 10% Pt they are visible a small area with agglomerations of nanoparticles. For CNT-20%Pt sample an agglomeration of Pt nanoparticles is dominated.

The carbon nanotubes is an interesting example of material with only s and p ($2s^2$ and $2p^4$) electrons contributing to the valence band. This consists of weak pi bonds originating from $2p_z$ orbitals and strong sigma bonding related to overlaps of 2s, $2p_x$ and $2p_y$ orbitals.

In Figure 2 the HeII spectra of clean CNT and graphite were compared. All spectra consists from five features, which can be assigned to C 2p π at 3 eV, overlaps (crossing) of C2p π and C2p sigma bands at around 5.5 eV and 7.8 eV, C2s-2p hybridized state at 10 eV and C2s band at about 13 eV [8]. Unfortunately, the strong peak at 6 eV originating from 2p electrons of oxygen atoms adsorbed on the surface of graphite limited visibility some features of the HeII spectrum of graphite.

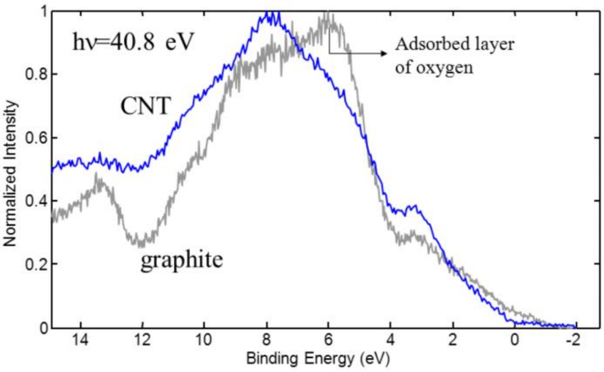

Figure 2. UPS HeII valence band spectra of CNT and graphite.

In Figure 3 the comparison of the HeII spectra corresponding to the valence band density of states (DOS) of pristine CNT and decorated by Pt nanoparticles were presented.

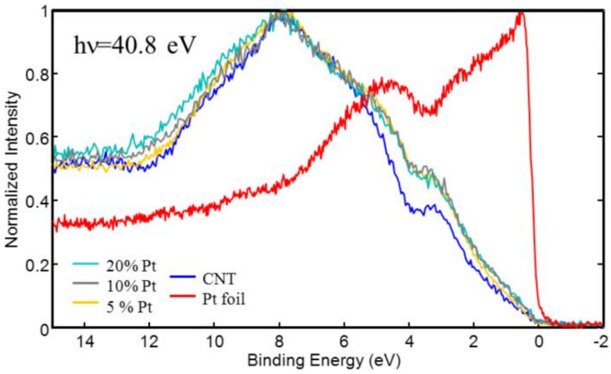

Figure 3. UPS valence band spectra of CNT, CNT-Pt and Pt.

These spectra exhibit visible changes in electron states below the Fermi level after being normalised to possess the same integrated intensity with respect to 0-15 eV of binding energies. In case of CNT decorated by Pt nanoparticles, increase of intensity 2p pi bands is clearly visible. Additionaly an increase of photoemission for hybridized C2s-2p states is visible, especially for 20% of Pt nominal doping.

In figure 4 a comparison of photoemission of examined samples was shown in the range –1 - 3 eV of binding energy.

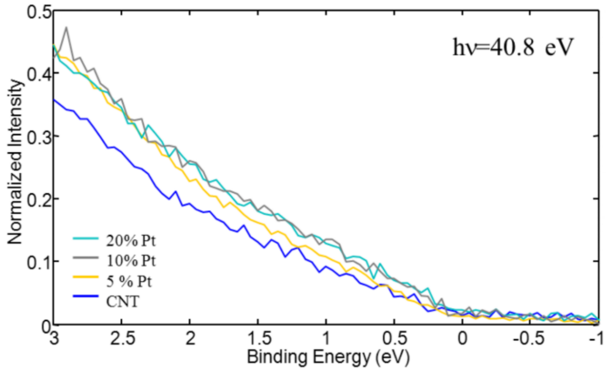

Figure 4. Intensity of photoemission near Fermi level.

An increase of density of states is visible for carbon nanotubes decorated by platinum nanoparticles. However, a small increase of photoemission signal near Fermi level observed in HeII spectra for CNT-Pt nanocomposite exhibit strong contrast with platinum HeII spectrum for which a high photoemission from 5d electrons is clearly visible in figure 3.

In figure 5 we presented the valence band spectra obtained by XPS method. As the nominal platinum content increases, the observed density of states at the Fermii level coming from the Pt 5d electrons also increases. A similar effect of increase photoemission was expected for UPS measurement. However, the observed increase in photoemission at the Fermii edge for CNT-Pt composites was very small.

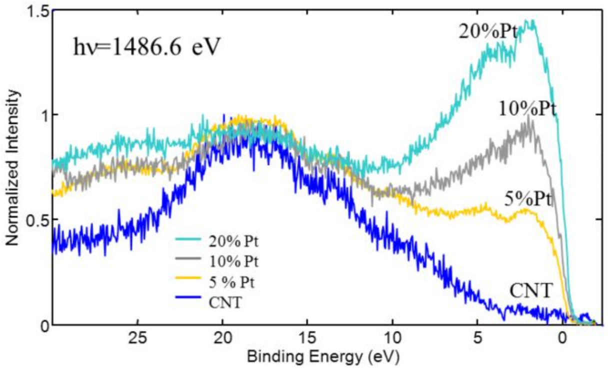

Figure 5. XPS valence band spectra of CNT nanocomposites.

In summary, we studied the electronic properties of clean CNT and decorated by Pt nanoparticles. We found a significant difference in photoemission from the pi band in relation to unmodified CNT material. The obtained results also demonstrate, that potential application in sensor of H2, CH4 and NO2 gases can be considered based on changes in density of states near Fermi level.

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P-06	**Monday, 04.09., 16^{30} – 19^{00}**

The possibility of synchrotron radiation use for CVD deposition of metals from their carbonyls – simulation

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It is known that the synchrotron radiation severely heats the filters and windows close to the ring [1]. That is why, the equipment requires permanent cooling. In this case, the heating effect of the synchrotron radiation (SR) is seen as unwanted effect.

It is proposed to use heat to produce the MEMS/NEMS (the micro/nano-electro-mechanical systems) using SR. This assumption makes sense, given the high brilliance and emittance of SR.

Some gaseous carbonyls of metals can be decomposed at low temperature in the 350-420 K range and can be used for deposition of metal to a substrate.

One of the most effective methods to obtain metallic micro/nanostructures from their carbonyls or halides is the laser chemical vapour deposition (LCVD) [2]. As an example, it is proposed to simulate the deposition of transition metals from their carbonyls to the dielectric substrate by laser CVD using the finite element method (fig 1). Parameters of the laser radiation at which the pyrolytic decomposition of carbonyls and deposition of the transition metals would be possible were determined as a result of calculation by finite element method.

The calculated profile of sediments of the transition metals (fig. 2, where are 1 - Cr, 2 - Co, 3 - Ni, 4 - Fe, 5 – Mn) was in good correspondence with the experimental data [3].

The model allows determining the sediment pattern during LCVD process and can be used with SR parameters, if SR is applicable to CVD deposition of metals.

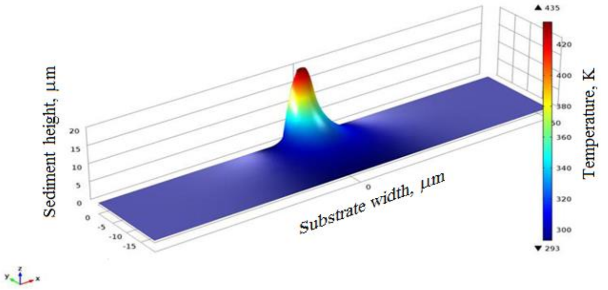

Figure 1. Temperature redistribution in the sediment.

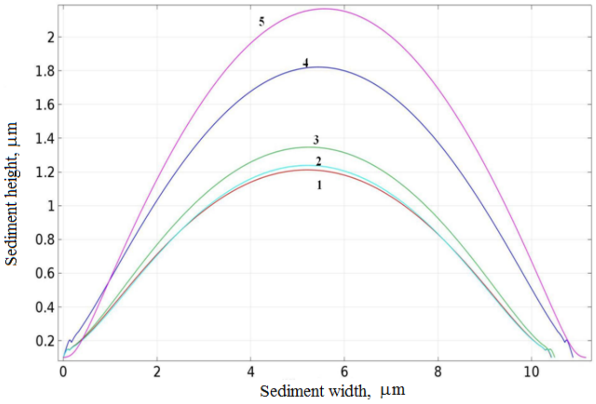

Figure 2. The profile of sediment after LCVD (2 seconds).

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P-07 **Monday, 04.09., $16^{30} – 19^{00}$**

Structural studies of amyloid beta peptide in solution of different type surfactants

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Keywords: small angle X-ray scattering, amyloid beta peptide, surfactants, circular dichroism, FTIR

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The most critical changes relevant to the progress of Alzheimer's disease (AD) are related to development and deposition of amyloid plaque whose main components are amyloid β-peptides (Aβ) [1,2].

The aim of our study was characterization of the structure and conformational changes of selected β-amyloid peptides (1-42 Aβ peptide and its shorter variants; N-terminal forms with hydrophilic properties and hydrophobic peptides from C-terminal fragment) in the presence of a wide group of surfactants. For this study four groups of surfactants (cationic, dicationic, tricationic and zwitterionic) were selected as well as the surfactant concentration effect was tested.

The secondary structure of Aβ peptides in the presence of different concentrations of surfactants, was tested using FTIR spectroscopy and circular dichroism (CD) methods. The size distribution of Aβ peptide aggregates was evaluated on the basis of complementary methods: gel electrophoresis and atomic force microscopy (AFM). AFM allowed also the visualization of Aβ assembly dynamics and Aβ fibril morphology. In presented research report we focused on resolving small oligomers [2] that are currently believed to initiate determination of the brain function in AD on defining stage oligomer to fibril growth by integration between optical spectroscopy determination of protein conformation and AFM observations.

A series of the small angle scattering of X-ray measurements using the synchrotron radiation (SR-SAXS) were performed for selected solutions of tested β-amyloid peptides with surfactants. The SAXS data for these surfactants were collected on P12 beam line of EMBL Hamburg Outstation on PETRA III storage ring at DESY. SAXS reveals globular structure of surfactant-Aβpeptide aggregates with can be involved in the chemical exchange and interact with hydrophobic or hydrophilic part of the peptides.

Acknowledgements: The study was supported by research grant „Grant Diamentowy'' from Ministry of Science and Higher Education (Poland) - DEC:0011/DIA2015/44.

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P-08 **Monday, 04.09., $16^{30} – 19^{00}$**

Local structure around erbium in the Er doped SiO_2/Si multilayers

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Various nanocrystalline silicon (nc-Si) structures, examined over last years, have been shown to exhibit efficient light emission in the visible region of the spectrum [1,2] which is associated with direct transition in Si quantum confined system. Silicon nanostructures doped with Er^{3+} have been found as a good candidate for an infrared efficient emitter at telecommunication wavelength (1535 nm). Indirect excitation of Er^{3+} ions via energy transfer mechanism from nc-Si to erbium is involved in this optical emission [3]. The key parameter in energy transfer process, which assures the efficient IR luminescence, is the distance between nc-Si (activator) and Er sensitize [4]. However, the mechanism is still under debate.

X-ray absorption fine structure (XAFS) techniques were applied in order to investigate local structure around the Er ions in the SiO_2:Er/Si layers fabricated by rf magnetron sputtering and subsequently annealed with various methods and temperatures. The studied layers were nm-thick and exhibited different photoluminescence spectra. Two series of samples were investigated. First with 1% of Er annealed at 900°C (rapid thermal processing (RTP) / furnace annealing (FA)). Second with 1, 3 and 5% of Er annealed at 1100°C (FA). The XAFS measurements were carried out at the Er L_3 edge. All samples were measured in a fluorescence mode with 12-element Ge detector. Additionally, reference Er_2O_3 powder sample was measured in a transmission configuration.

Extended X-ray absorption fine structure (EXAFS) analysis reveals that the first sphere in all cases consist mainly of oxygen atoms. The nearest neighbourhood does not substantially differ between the considered samples; however, some differences can be observed. X-ray absorption near edge structure (XANES) calculations were performed for several crystal structures in order to check the shape of the spectra for possible Er neighbourhoods. Results of the XAFS investigation were correlated with the photoluminescence studies.

Acknowledgements: The XAFS experiments were performed on beamline LISA (BM08) at the European Synchrotron Radiation Facility (ESRF), Grenoble, France. We are grateful to Dr. Francesco d'Acapito at the ESRF for providing assistance in using beamline. H.K. acknowledges financial support through from the Army Research Office (ARO) under contract W911NF-14-1-0290.

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P-09 **Monday, 04.09., $16^{30} – 19^{00}$**

Local structure of Co and Mn dopants in Bi_2Te_3 single crystals

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Bi_2Te_3 single crystals belong to the class of materials called Topological Insulators (TIs). These are insulators in the bulk with surface states protected by time reversal symmetry that is, resistant to impurities, defects, and geometry deformations. The correlation between electronic and magnetic properties of TIs modified by magnetic and non-magnetic bulk doping and its influence on topological transport properties is of great importance in order to tailor the key materials properties in terms of application in spintronics.

Among crystalline TIs the long range magnetic order is established only in the Mn-doped Bi_2Te_3 in the temperature range below $T_C = 12$ K. On the other hand, in iron and cobalt doped bismuth chalcogenides, long range magnetic order has not been observed, while magnetic susceptibility reveal intriguing anizotropy, that is tentatively ascribed to non-uniform distribution of transition metal dopants between cation sites of Bi and interstitial position within van der Walls (vdW) gap.

Our goal was to probe the distribution of Co and Mn magnetic dopants in the crystal structure of single crystalline samples of Bi_2Te_3 in order to establish the preferential doping sites and relate it to the unique magnetic properties of these materials. The goal was achieved by means of Extended X-ray Absorption Fine Structure (EXAFS) and Angle Resolved X-ray Absorption Near Edge Structure (AR XANES) spectroscopies.

Acknowledgements: Supported by National Science Centre, Poland (grant number: 2015/17/B/ST3/00128.

P-10 **Monday, 04.09., $16^{30} – 19^{00}$**

High temperature structure evolution of (Ga, Mn)As compound: *in-situ* diffraction study

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Searching the new materials with properties combining both ferromagnets and semiconductors is the most pressing problems of spintronics. One of the most studied material among diluted magnetic semiconductors (DMS) is (Ga, Mn) As [1]. The existing RKKY theoretical model [2] predicts an increase of the Curie temperature (TC) with increasing concentration of specific dopants [3], which is not always confirmed by the experiment. The optimized MBE growth and post-growth annealing procedures yield (Ga, Mn) As layers of TC as high as about 200 K [4]. This value is quite high as for DMS, but still too low in view of potential application in spintronic devices. To understand dynamical processes taking place in structure evolution of (Ga, Mn) As during growth and postgrowth annealing, it is very important for the purpose of further progress in TC increasing of (Ga, Mn) As. In our previous investigations we have shown that the TC increase in (Ga, Mn) As upon LT post growth annealing is correlated with the decrease of the lattice parameter [5]. We also showed [5] that the optimum LT post-growth annealing is a subtle process, since (Ga, Mn) As is a metastable compound (it starts to decompose at temperatures only slightly higher than the growth temperatures). Extended annealing at temperatures above 300°C leads to diffusion of Mn from Ga sites and formation of Mn rich (MnAs) clusters in GaAs matrix of the former (Ga, Mn) As layer. Further annealing at temperatures higher than about 470°C lead to an increas the lattice parameter of the layer, again. In (Ga, Mn) As annealed at these and higher temperatures, the segregated MnAs nanocrystals have been detected by transmission electron microscopy [5]. But the structure of these MnAs nanocrystals is not determined yet.

In the presentation we will investigate structure evolution and temperature stability of relaxed (Ga, Mn) As samples during in-situ HT-annealing (up to about 500°C) by X-ray powder diffraction. The samples were grown by means of the LT-MBE technique at temperature of 230°C and detached from the GaAs substrate. We will show the (Ga, Mn) As lattice parameter temperature dependence as well as retrace MnAs -type nanoclusters created by annulling action in these materials and dynamic of their temperature structure evolution.

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P-11 **Monday, 04.09., $16^{30} – 19^{00}$**

AFM and XPS studies of impact of the surface oxidation on the properties of Bi_2Te_3 thin films

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Topological Insulators (TI), a novel class of quantum materials [1] are considered as promising materials for multiple applications in next generation electronic or spintronic devices. The existence of metallic surface states on insulating bulk is the most important feature of this class of materials. However it is well known that defects, strains and doping influence that important feature of the TI's. In our studies we focused on impact of surface oxidation on properties of one of known TI's - Bi_2Te_3.

We used X-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM) to study behavior of Bi_2Te_3 films of different thicknesses exposed to the atmosphere. With the use of MBE system we have grown step-like sample with thicknesses of particular Bi_2Te_3 layers ranging from 40 to 100 Å. The sample was grown on mica substrate in the co-deposition mode as described in our previous work [2]. The electron diffraction measurements (RHEED) confirmed monocrystalline structure of the film. The studies of electronic structure, focused on the analysis of the Bi4f, Te3d and O1s core levels, were realized after the deposition and after the oxidation process. The results indicate formation of Bi_2Te_3 compound, and further, after exposition to the air the oxidation of the film surface. The AFM measurements realized after oxidation process revealed grainy structure of deposited films and thickness dependent changes of the surface roughness ranging from 0.3 to 2.25nm. Additional features as presence on selected films of fusiform grains, channels and craters were detected.

Acknowledgements: This work was supported by Research Grant NCN 2016/21/B/ST5/02531.

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P-12 **Monday, 04.09., $16^{30} – 19^{00}$**

Fluorescence studies of photoexcitation and decay of the $2p^{-1}nl$ core-excited states of Ar atoms

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The core-excited states of argon produced by excitation of the 2p electron into the ns and nd Rydberg orbitals appear as peak structures below the $2p^{-1}\,{}^2P_{3/2,1/2}$ ionization thresholds in photoabsorption [1], electron energy-loss spectra [2] and photoionization [3] spectra. The $2p^{-1}nl$ states decay predominantly via resonant Auger transitions that populate valence-excited $3p^4({}^3P,{}^1D,{}^1S)nl$ states of the Ar^+ ions. The excited Ar^+ ions further decay by emission of the UV-VIS fluorescence or directly to the ground ionic state by UV emission. The UV-VIS emission is generated via radiative cascades [4], what complicates the interpretation of the fluorescence spectra and different techniques are required to study the decay dynamics.

In this communication we present the fluorescence studies of photoexcitation and decay of the $2p^{-1}nl$ core-excited states of Ar atoms using the photon-induced fluorescence technique [5] combined with a photon-photon delayed-coincidence detection system. In particular, we have used the photon induced fluorescence technique to measure fluorescence yield spectra of the $3p^4({}^1D)5s({}^2D) \rightarrow 3p^4({}^1D)4p({}^2F)$ (393 nm) and $3p^4({}^1D)4d({}^2F) \rightarrow 3p^4({}^1D)4p({}^2F)$ (335 nm) emission lines over the energy range of 240-255 eV (Figure 1). We have also utilized the photon-photon delayed-coincidence system in order to observe events where the decay of the 2p inner shell excited argon in the 240-255 eV energy range leads to the emission of two UV/visible photons. The coincidence measurements have been performed for the 335/459 nm and 393/459 nm emission cascades (shown in Figure 2) at various photon energies across the Ar 2p excitations. For those cascade transitions the delayed coincidence photon decay curves have been measured over the energy range of excitation of the $2p^{-1}nl$ states of argon. The lifetimes of the $3p^4({}^1D)4p({}^2F_{7/2,5/2})$ states of Ar^+ as well as the coincidence yield spectra have been determined from the obtained curves.

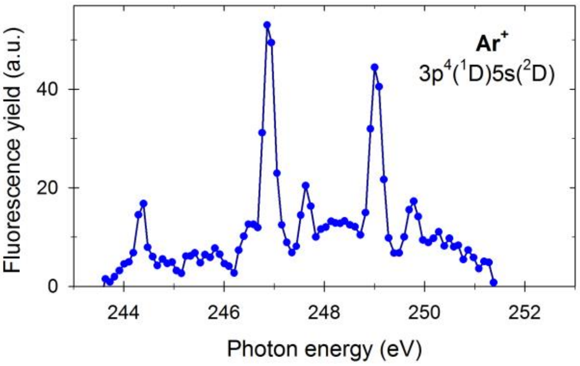

Figure 1. Fluorescence yield of the 5s(2D) state.

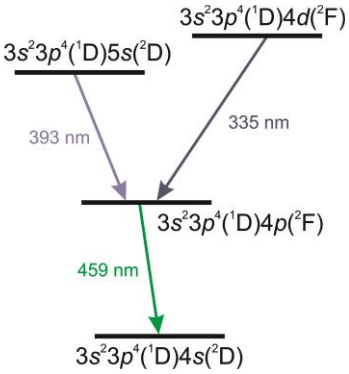

Figure 2. Diagram of fluorescence cascade transitions.

Acknowledgements: This work was financially supported under the CALIPSO contract.

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P-13 **Monday, 04.09., 16^{30} – 19^{00}**

Structural changes of Co-implanted ZnO single crystals as a function of Co concentration and annealing temperature

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Zinc-oxide (ZnO) crystals doped with transition metals (TM) were theoretically predicted to exhibit room-temperature ferromagnetism [1, 2]. The origin of ferromagnetism in ZnO:TM is attributed to the presence of TM atoms at Zn sites (so called diluted magnetic semiconductor (DMS)), the existence of TM-containing secondary phases, and the precipitates of TM nanocrystals. The ion implantation is one of the widely-used methods for the incorporation of TM into ZnO crystals. However, the major drawback of the implantation are heavy damages of the crystal lattice caused by the radiation of high-energy ions. Therefore, in order to restore a high quality of the crystal lattice, the thermal treatment of the post-implanted sample is required. Such a treatment quite often may lead to the formation of secondary phase precipitates, especially in samples implanted with relatively high doses of TM. These precipitates may have considerable impact on magnetic properties of the implanted material.

In this contribution, we report X-ray diffraction (XRD) structural investigations of ZnO(0001) single crystals implanted with different concentrations of Co ions: 10%, 14%, 16%, 18% and 22% with respect to the Zn and O ions. The thickness of the implanted layers (250 nm) was calculated from the appropriate values of ion energies and fluences used during the implantation process. The XRD structural characterization was performed using synchrotron radiation at the BM25 beamline at the ESRF, the European Synchrotron. The energy of the monochromatic X-ray beam was set to 22.037 keV and a 2D MaxiPix detector was used for the data collection.

To resolve the structure of the implanted crystals, a set of 2θ -ω X-ray diffraction patterns were collected from the as-implanted samples and after subsequent cycles of annealing at 900ºC and 1200ºC. The aim of such a procedure was ascertainment the thermally induced formation of new crystallographic phases, and their temperature stability.

The analysis of the experimental data revealed a partial substitution of Zn ions by Co ions in the lattice of as-implanted host ZnO crystals, resulting in the formation of the $Zn_{1-x}Co_xO$ solid solution inside the implanted layers. After annealing at 900ºC, except for the sample with 10% Co concentration, the thermally stable secondary phase, spinel-type $ZnCo_2O_4$, is formed. Significant structural changes in the implanted layers are observed after annealing at 1200ºC. The previously identified phases, $Zn_{1-x}Co_xO$ and $ZnCo_2O_4$ are absent, and a new, not recognized phase appears.

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P-14 **Monday, 04.09., 16^{30} – 19^{00}**

Valence-change-induced Fano resonance: RPES of Yb implanted ZnO

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RE-ion doped semiconductor materials are particularly interesting for infrared (IR) emitting optoelectronic devices due to their intra-4*f* shell transitions in the 1.4-1.7 μm range [1-2]. In addition, with visible emission from higher excited levels (green for Er, Yb), they potentially can be used in devices such as optical amplifiers, lasers and optically pumped glass fibers [3]. For this, it is important to understand the RE ions fundamental properties in wide band gap semiconductors, such as their lattice site locations and surroundings, and the optical ion activation mechanisms and emission properties.

The resonant photoemission (RPES) experiment was used in this project to investigate the ytterbium electronic states and their hybridization with valence electrons of zinc oxide. The measurements were performed at Elettra synchrotron facility (Trieste, Italy). The obtained data were used to establish the correlation between the optical properties and the electronic structure. Both commercial single ZnO crystals and epitaxial ZnO films grown at IP PAS by Atomic Layer Deposition (ALD) technique were under investigations. Ytterbium ions were incorporated into the ZnO matrix via ion implantation and subsequent annealing. We investigated samples containing different quantity of (co-)doped RE atoms (implantation of Yb at the level of 10^{15} and 10^{16} cm^{-2}). Prior to photoemission experiments, Ar^{+} sputtering and annealing of the investigated samples up to ~573 K were performed. Photoemission spectra were taken for the photon energy range 180-190 eV i.e. across the Yb4*d* – Yb4*f* photoionization threshold which allows observation the Fano resonance enhancement from the Yb4*f* electron shell.

In RPES the photon energy is tuned to the inter-ion absorption resonance (in our case Yb $N_{5,4}$) providing an interfering channel for a classical photoelectron excitation. As a result, the photoemission intensity dramatically increases or decreases, depending on the relative amplitudes and phases of the interfering channels. This effect is applied to derive the contributions of the Yb4*f*electron states to the valence band of the measured system. We found a inconsiderable but clear resonant enhancement of Yb4*f* states to the ZnO:Yb valence band at binding energy about 7.5 eV below the Fermi level. A weak Fano resonance is consistent with a large $4f^{14-\delta}$ occupancy. It was also found that ytterbium 4*d* level shows an extended multiple structure instead of a simple spin-orbit doublet for metallic ytterbium, which allows concluding that majority of ytterbium atoms are bonded to oxygen and indicates that one of the $4f^{14}$ electrons has been promoted to the valence level. This multiple structure can be attributed to $4f^{n} \rightarrow 4d^{9}$ interaction.

The obtained results enhance our general understanding of RE ions fundamental properties and are of great importance to the development of optical devices as well as devices used in short-range high speed networks operating in the IR.

Acknowledgements: The work was supported by the Polish National Centre for Research and Development (NCBiR) through the project PBS2/A5/34/2013, partially supported by the EAgLE international project (FP7-REGPOT-2013-1, Project No. 316014), and the international project co-financed by Polish Ministry of Science and Higher Education, Grant Agreement 2819/7.PR/2013/2.

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P-15 **Monday, 04.09., 16^{30} – 19^{00}**

Small angle X-ray scattering studies of the full length human prion protein in different pH conditions

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Human prion protein (huPrP) is a small 28 kDa membrane glycoprotein anchored in the phospholipid bilayer via glycophospatidylinositol and this protein is implicated in the pathogenesis of serious neurodegenerative disorders (transmissible spongiform encephalopathies - TSEs) [1]. This protein consists of an unstructured domain at the N-terminus, which contains four octapeptide repeats and C-terminal, alpha helical domain stabilized by the disulfide bridge. The above mentioned octapeptide repeats are involved in binding of copper ions as well as other divalent metal ions [2,3]. Despite the fact, that about 20 years of structural studies of human prion protein resulted in solution of partial structure of this protein and its homologs from other organisms (i.e. hamster or bovine), the mechanism of conversion of cellular form (huPrP^{C}) into pathological scrapie form (huPrP^{Sc}) has not been fully understood yet [1,4-10]. Also the impact of metal binding on the overall conformation and structure of huPrP^{C} is not fully known.

The aim of our studies was characterization of structure in solution of human prion protein variant (cellular form) and its conformational changes in different environments. In this presentation we report preliminary data concerning conformation and structure of the huPrP^{C} protein in solution at various pH conditions studied using small angle X-ray scattering (SAXS). The SAXS experiments were performed using synchrotron radiation (DESY, PETRAIII) as well as the SAXS data were collected by the use of XEUSS 2.0 system using X-rays generated by a lab source (MetalJet microfocus generator). The obtained scattering data were used for modelling of low resolution structure in solution, which will be presented.

Acknowledgements: This work was supported by National Science Centre, Poland, under grant No. 2014/15/B/ST4/04839.

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P-16 **Monday, 04.09., 16^{30} – 19^{00}**

On the influence of nanostructurization on the shape of K pre-edge in iron oxides

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Size and shape of material greatly influence its electronic structure and thus material's functional properties relevant for applications in e.g. spintronic [1]. Lowering material's dimension and introducing collateral damage to outer layers by means of nanostructurization enhances the impact of surface states and changes the volume properties, e.g. magnetic anisotropy. Understanding those processes and how they influence the properties known from bulk samples, cannot be achieved without the knowledge on structural defects, especially of those related to nanostructurization.

Using HERFD XAS technique we measured local structure and electronic configuration of iron in different types of nanoscale oxide samples formed from magnetite, maghemite and/or hematite. Thin epitaxial layers obtained by means of PLD, nanostructured by either electron lithography combined with ion etching or direct lithography using Focused Ion Beam, nanocomposites obtained with magnetron sputtering and nanoparticles in solution were studied at the ID26 beamline at ESRF.

HERFD XAS is a sensitive probe of local atomic environment. It is especially favorable in resolving the pre-edge structures, that are sensitive mainly to crystal field symmetry and formal valence of the ensemble of metal ions [2]. The experimental results show, that in general, the evolution of XAS spectra of nanoscale iron oxides can be divided in two types, based on pre-edge shape evolution. The first type is related to the main pre-edge peaks, which resembles either magnetite (single peak), hematite (double peak) or maghemite (single peak with energy shift) [3]. The second type are samples after nanostructurization treatment, that show additional peaks at the high energy side of the pre-edge range, tentatively attributed to distortion of the local structure [4]. Information from pre-edge area is compared to the main edge. The latter remains intact in shape for most of the studied samples. Its shape resembles the one known from magnetite spinel structure, but is shifted in energy, suggesting different oxidization state of iron, namely a variable proportion of Fe3+ and Fe2+ ions in the samples [3].

Acknowledgements: This work was supported by National Science Center of Poland (grants: 2014/14/E/ST3/00026 and 2015/17/D/ST3/00968).

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P-17 **Monday, 04.09., $16^{30} – 19^{00}$**

Human Cystatin C in trimeric form - molecular dymanic, SAXS, SANS and NMR studies

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Amyloid formation is the mechanism associated with the development of many neurodegenerative disorders. However, despite increasing knowledge of particular diseases like Alzheimer’s, Huntington’s or Parkinson’s, the issue whether the amyloid fibrils, being the final stage of aggregation, or the intermediates in the oligomerization process, are the origin of toxic effects is still under debate. Therefore, the developing of effective therapeutics is compromised by the difficulty in accurately defining toxic species. Thus, study of amyloidogenic proteins that, at some conditions, or due to some mutations, are prone to aggregation is extremely important. Within this study, our intend was to characterize structurally one of oligomeric states of an amyloidogenic protein, particularly the trimeric from of human cystatin C (HCC).

HCC is a small protein, an inhibitor of sulfhydryl proteases, that can form a number of oligomeric forms in solution (e.g. dimers, trimers, tetramers, decamers and other higher oligomers) [1,2]. HCC acts as inhibitor in monomeric form, but the best-known crystal form of cystatin C is the dimer, which is formed via a domain-swapping mechanism, in which one fragment of a HCC monomer is exchanged with its counterpart from another HCC molecule [3]. It is postulated that throughout this mechanism (propagated domain-swapping) higher HCC oligomers are formed, eventually leading to the formation of HCC amyloid deposits. This protein was also detected as codeposite in the amyloid plaques of Alzheimer's disease or Down's syndrome. Additionally, its point mutant (L68Q variant) is the cause of fatal cerebral amyloid angiopathy in early adult life [4-5].

To investigate the structure of the selected HCC oligomers, we used a covalently stabilized trimer of HCC. We established a low-resolution structure of the HCC trimer based on the experimental small angle X-ray scattering of synchrotron radiation (SAXS) data and ab initio modelling. As a result of molecular docking and molecular dynamics simulations studies we proposed the atomic model of HCC trimer. The structural parameters of this molecule in solution were also verified by small angle neutron scattering (SANS) and nuclear magnetic resonance (NMR) diffusometry. The most stable model of the three-dimensional structure of HCC trimer obtained from the molecular dynamics simulation is characterized by well-preserved elements of secondary structure and reproduces well the overall molecular shape.

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P-18 **Monday, 04.09., 16^{30} – 19^{00}**

Spectrometric analysis of the rare earth niobates

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The rare earth niobates have recently been investigated as novel protonic conductors. Their chemical formula is RE_3NbO_7, where RE is the rare earth metal (Y, La, Ce...). These compounds crystalize in defected fluorite structure, where oxygen vacancies randomly occupy the anion site. Filling the oxygen vacancies with OH^- protonic defects, should increase the total conductivity in this material. This protonic incorporation may lead to decrease the level of activation energies. Hence the rare earth niobates could be applied as a good solid electrolyte in the protonic ceramic fuel cells (PCFCs).

Therefore XPS investigations were performed on yttrium niobate Y_3NbO_7 and titanium doped yttrium niobate $Y_3Nb_{0.85}Ti_{0.15}O_{7-\delta}$ in order to provide suitable information for further detailed chemical and physical analysis.

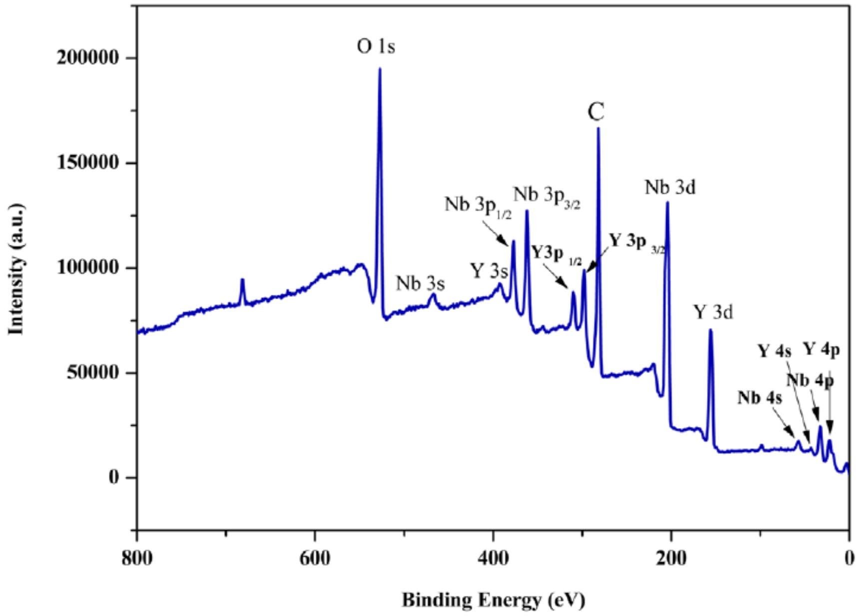

Figure 1. The survey spectrum of Y_3NbO_7 [5].

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P-19 **Monday, 04.09., $16^{30} – 19^{00}$**

Application of XES and XAS to study doped TiO_2

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Within growing demand for energy, the world industry is forced to seek for new solutions based primarily on renewable energy sources. One of the main goals is the use of solar irradiation to supply energy and to initiate chemical reactions by photocatalysis. The problem is finding the efficient material - a photocatalyst, which promotes the reaction using light from the visible range. Unfortunately, titanium dioxide that is very active and efficient catalyst works only in the UV range. The solution is modification of the electronic structure (band gap reduction) to induce visible light activity by doping with 3d elements such as V, Cr, Mn, Fe, Co and Ni, which shifts the conduction band downwards in energy or light elements such as N, S and C able to shift the valence band upwards in energy [1,2].

Previously published work are mainly based on studies confirming the increase in the absorption of visible light by the use of doping but their impact on the electronic states of the photocatalyst is still being discussed. In this work, using X-ray spectroscopy methods such as

X-ray emission (XES) and X-ray absorption spectroscopy (XAS), we present the influence of Cr and N doping on the TiO2 electron structure. Thanks to the combination of XES and XAS spectroscopy (see Fig. 1), we investigate the density of occupied and unoccupied states in the atom and the effect of dopants on the formation of valence and conduction bands of photocatalysts. The doping effect on electronic states is further confirmed with calculations involving N- and Cr-doping by means of FEFF9.0 program. The calculated density of states for Cr-doped TiO2 reveals twofold influence on electronic state composition. First the Ti 3d-band is slightly damped in intensity by about 5%, but keep the doublet d-band structure as in case of pure TiO2. Secondly, a new electronic orbital is introduced on the low energy side of unoccupied electronic states that corresponds to Cr d-band [1]. The N-doping induces the shift of valence states to higher energies and thus leads to the band-gap narrowing. Simultaneously, conduction states do not show any N-doping induced effects. The band-gap narrowing is mostly due to the N 2p electronic states being introduced to the valence band on the high-energy side.

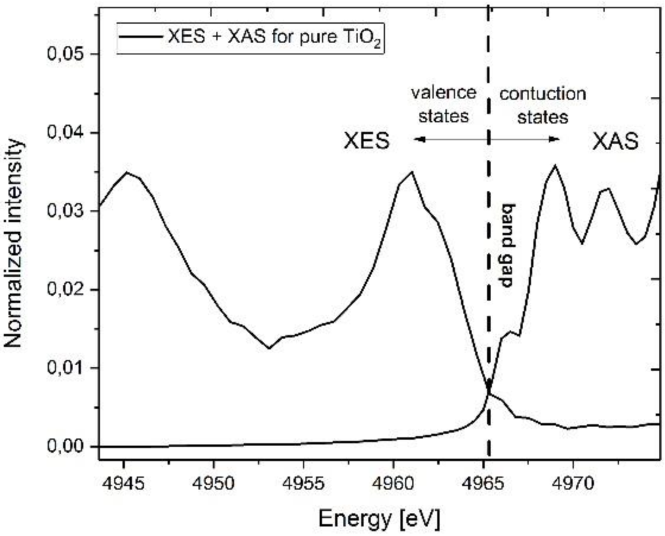

Figure 1. Experimental results for XES/XAS spectra for TiO_2.

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P-20 **Monday, 04.09., 16^{30} – 19^{00}**

Two Photon Absorption (TPA) process at hard X-ray energies

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Standard and well known X-ray spectroscopy is based on one photon absorption and one photon emission processes, where the signal is linearly dependent on the incidence radiation intensity. However, when the intensity of the radiation beam is high enough, it is possible to observe the effects based on multi-photon interactions with matter. It this case, the signal is nonlinearly dependent on radiation intensity. In the optical region, of the electromagnetic wave spectrum the nonlinear photon-matter interactions are observed since the development of the high intensity ruby laser in the 1960 [1], [2]. The possibility of investigating the nonlinear phenomena at hard X-ray regime was a technical problem until now, since lack of the source of X-ray's that could provide the sufficient beam intensity, to induce nonlinear interactions in the matter. Thanks to the recent development of X-ray Free Electron Lasers (XFEL) is it possible to reach the high enough beams intensities, being essential in order to investigate the nonlinear X-ray – matter interactions [3].

The main difference between the optical and the X-ray interactions with matter is the possibility of direct excitation of the electrons on the atomic core shells, which can result in creation of the intermediate states with lifetimes lower than 1 fs [4]. Using the femtosecond radiation pulses from XFEL's, opens an opportunity to research the yet unexplored area of physics, and investigate the mechanism which lead to the nonlinear X-ray-matter interactions [5].

The two photon absorption process (TPA) makes possible to observe the different excited atomic states, thanks to the selection rules. Unlike in the one photon absorption, which is defined by dipole selection transitions, the TPA process requires the change of orbital quantum number by +/-2 or 0. This feature, allows observing thus the electronic transitions that are forbidden in linear regime, as well as to probe yet undiscovered electronic states. Practical use of two photon absorption process with XFEL's is still problematic. This is because of the low cross-sections value for TPA processes, so it competes with the photon-atom interaction mechanisms of primary and secondary order. This has to be taken into account with the use of very short radiation pulses. Therefore, knowledge of time evolution of atomic state populations during course of femtosecond X-ray pulse is essential for deep understanding of mechanisms leading to two photon absorption.

Herein we compare the experimental data for one and two photon absorption obtained with the LCLS X-ray free electron laser (published in [5]), with the computations performed for time-dependent states population for these processes. The absolute X-ray rates as well as states populations are computed within three level atomic model. The results shows states narrowing for nonlinear interaction as a result of square dependence on incidence X-ray intensity.

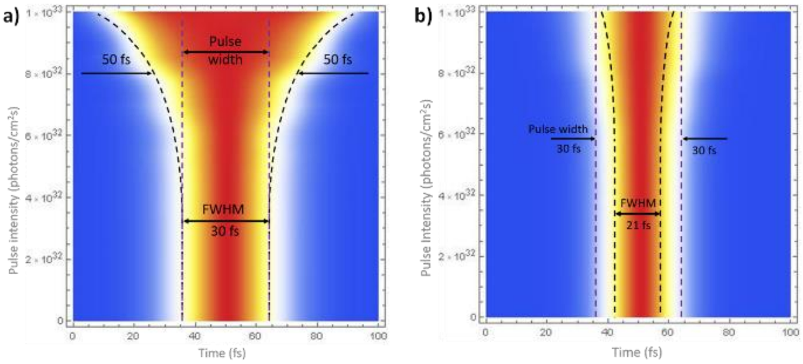

Figure 1. Temporal profiles for OPA (a) TPA (b) processes.

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P-21 **Monday, 04.09., $16^{30} – 19^{00}$**

Resonant Fano type photoemission to study of RE 4f electrons contribiution to the valence band

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The synchrotron radiation source was used to extract the range of energy from 30 to 200 eV and apply it to study contribution of rare earth (Eu, Gd, Sm) 4f electrons to the valence band of semiconductors electronic structure.

In the regular photoemission the photon of energy hν = 4f – 4d leads to the photoemission of electron 4f:

$$\mathrm{Eu}\ 4d^{10}4f^{7} + h\nu \rightarrow \mathrm{Eu}\ 4d^{10}4f^{6} + e^{-}$$

In Fano type [1,2] resonant photoemission the same energy of hν photons is absorbed (transition 4d -4f) and resonant interaction leads to emission of additional 4f electrons:

$$\mathrm{Eu}\ 4d^{10}4f^{7} + h\nu \rightarrow (\mathrm{Eu}\ 4d^{9}4f^{8})^{*} \rightarrow \mathrm{Eu}\ 4d^{10}4f^{6} + e^{-}$$

This additional emitted electrons create new structure of the density of states corresponding to 4f electrons structure.

The presented results are concern to the study of the change of the semiconductor valence band density of states structure caused due to interaction and contribution of 4f electrons states to the total semiconductor valence band. The impurity RE (Eu, Gd, Sm) atoms were introduced into the volume of the crystal or sequentially deposited on the crystal surface. Measured spectra showed the curves with the contribution of the electrons 4f corresponding to valence 2+ or 3+. For temperature annealing of the samples the change of their valence was observed.

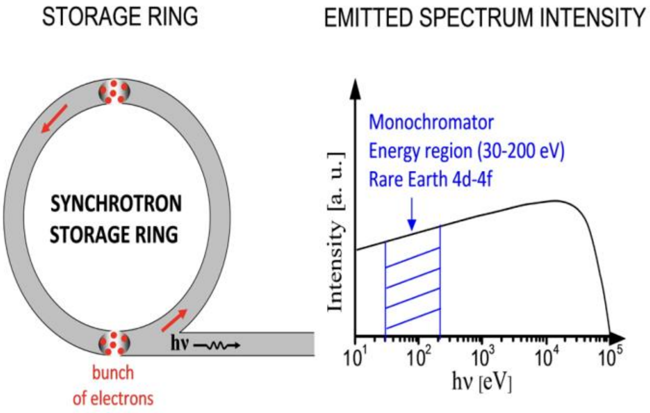

Figure 1. Synchrotron ring with emitted spectrum intensity.

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P-22 **Monday, 04.09., 16^{30} – 19^{00}**

The synchrotron powder XRD and periodic DFT studies on the pressure behavior of katoite

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Katoite, $Ca_3Al_2(SiO_4)_{3-x}(OH)_{4x}$ (x=1.5-3) is a mineral belonging to garnet family, crystallizing in regular system (*Ia3d*). It is supposed to be one of the main water bearing minerals in Earth mantle, and the pure aluminum katoite is the only thermodynamically stable calcium hydroxyaluminate phase in hydrated cements. Hence the understanding of mechanistic properties of katoite is of great importance in both Earth science and civil engineering. Whereas several studies, both experimental and theoretical, on the pressure behavior of stoichiometric pure Al katoite exist [1, 2], little is known about the influence of Al substation on katoite compressibility.

The high pressure behavior of iron doped katoite, $Ca_3Al_{1.7}Fe_{0.3}(OH)_{12}$ is presented here [3]. Synchrotron powder X-ray diffraction measurements were performed in ALBA synchrotron (Barcelona, Spain) for the samples of pure Al and Fe doped katoite in the pressure range up to 10 GPa. Bulk modulus was estimated from the fitting of pressure-unit cell volume curve to the third order Birch-Murnaghan equation. The substitution of Al by Fe ions lowered the bulk modulus in comparison to Fe-free katoite. The softening of katoite upon Fe doping was explained by the density functional theory calculations as the effect of the change in hydrogen bond network, accompanied by the weakening Ca-O bonds and the increased compressibility of the latter ones.

Acknowledgements: This work has been supported by (1) Spanish MINECO through BIA2014-57658-C2-1-R and BIA2014-57658-C2-2-R, which is cofounded by FEDER, research grants, (2) PL-Grid infrastructure, (3) the EAgLE international project (FP7-REGPOT-2013-1, Project No. 316014) and the international project co-financed by Polish Ministry of Science and Higher Education, Grant Agreement 2819/7.PR/2013/2, (4) Project FIS2013-48286-C2-1-P of the Spanish Ministry of Economy and Competitiveness MINECO, the Basque Government under the ETORTEK Program 2014 (nanoGUNE2014), and the University of the Basque Country (Grant No. IT-756-13). We also thank CELLS-ALBA (Barcelona, Spain) for providing synchrotron beam time at BL04-MSPD.

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P-23 **Monday, 04.09., $16^{30} – 19^{00}$**

Charge density waves and hidden nesting in $K_xP_4W_8O_{32}$ and $P_4W_{12}O_{44}$ bronzes

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The members of the quasi-low dimensional monophnosphate tungsten bronzes (MPTB) family are known to exhibit the Peierls transitions towards the charge density wave (CDW) state [1]. The low dimensional character of MTPB arises from their crystal structure constructed of infinite conducting W-O slabs separated by insulating P-O layers in which the pentagonal tunnels are formed. Upon the intercalation of alkali metal atoms, the tunnels become hexagonal. Despite the CDW character of the phase transitions in the former group was undoubted, the nature of the crossovers seen in bronzes with hexagonal tunnels was questioned. To explore the impact of the the phase transitions on the physical properties of MPTB, we have selected two members of this family: $K_xP_4W_8O_{32}$ with hexagonal tunnels and $P_4W_{12}O_{44}$ with pentagonal tunnels.

For $K_xP_4W_8O_{32}$, we have performed an extensive analysis of transport, thermoelectric, magnetoresistance and magnetic properties and proven the condensation of the part of the electronic carriers and the opening of the CDW in the conduction band. These results, combined with the high resolution X-ray diffuse scattering study using synchrotron radiation allowed us to unambiguously identify this transition as a genuine Peierls instability [2].

The second compound, $P_4W_{12}O_{44}$ shows a series of three CDW transitions. We have investigated the formation of the superstructure accompanying them in the means of X-ray diffuse scattering experiment performed with synchrotron radiation. To complement the diffraction experiment we have studied the Nernst effect, which shows giant features due to reduction of electronic density and increase of carriers mobility caused by consequent Fermi surface nesting accompanying the cascade of the Peierls instabilities [3].

Acknowledgements: Financial support by the French National Research Agency ODACE ANR-Project No. ANR-11-BS04-0004 is gratefully acknowledged.

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P-24 **Monday, 04.09., $16^{30} – 19^{00}$**

Surface characterization of bismuth-lead-silicate glasses by X-ray Photoelectron Spectroscopy method

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The silicate matrix in pure silicate glasses presents relatively large phonon energy (about 1200 cm^{-1}) and low refractive index (about 1.5) [1]. The introduction of Bi_2O_3 into these glasses leads to lower phonon energy, larger refractive index, longer emission lifetime and better gain property [1]. These properties make bismuth-silicate glasses an interesting material for various applications, e.g. IR transmitting agents, low-loss fibre optic or as an active medium in Raman fibre optical amplifiers [2]. Although their applicability is limited mostly due to a very low electrical conductivity, it can be increased in a process of bismuth-silicate glass reduction performed in hydrogen. It has been noticed previously that within this process a reduction of bismuth ions takes place and the formation of metal grains both in an amorphous glass matrix and on the glass surface becomes visible [2]. Moreover, after the reduction in hydrogen Bi-Si-O glasses exhibit high electron secondary emission (up to 8–10 orders of magnitude higher than unmodified glasses) and can be used in the production of electron multiplier devices in the form of single channeltrons and micro-channel plates (MCPs) [3].

Lead-silicate glasses, due to their specific and very interesting properties, find a lot of industrial applications. As special materials, they are used in the production of plate image amplifiers and scintillators [3]. Lead-silicate glasses submitted to the reduction process (e.g. in hydrogen atmosphere), undergo dramatic changes of optical properties [4] and electrical surface conductivity, and reveal a very high secondary emission coefficient, thus also finding applications in the production of electron channel multipliers [5]

Mixing several oxides of large, polarisable cations, such as Bi_2O_3 and PbO, tends to stabilise the glasses and/or lower the required amount of true network formers. To our best knowledge there is still lack of evidence about the influence of heating and reduction in H_2 on the atomic structure of partially reduced Bi_2O_3-PbO-SiO_2 glasses.

The aim of this paper is to analyze the surface properties and structure of reduced bismuth-lead-silicate glasses. For this reason four compositions of glasses with different Bi/Pb molar ratio were prepared: xBi_2O_3-(30-x)PbO-$70SiO_2$, where x = 2, 5, 10 and 15. A structure and phase composition will be analyzed using the X-ray Difftraction (XRD) method, whereas the atomic structure will be analyzed by the X-ray Photoelectron Spectroscopy (XPS) technique.

Acknowledgements: This work was supported by the National Science Center under the grant No. NCN 2016/21/B/ST8/03193.

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P-25 **Monday, 04.09., 16^{30} – 19^{00}**

Laserlab-Europe Project

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Lasers and photonics, one of only five key enabling technologies identified by the European Union, are essential for the scientific future as well as for the socio-economic security of any country. Given the importance of lasers and their applications in all areas of sciences, life sciences and technologies, Laserlab-Europe - The Integrated Initiative of European Laser Research Infrastructures project has been established under the Horizon2020 program (https://www.laserlab-europe.eu/). The project brings together 33 leading institutions in laser-based inter-disciplinary research from 16 countries. Together with associate partners, Laserlab-Europe covers the majority of European member states.

Laserlab-Europe is a member of the European Cluster of Advanced Laser Light Sources (EUCALL). EUCALL is a network between leading large-scale user facilities for free-electron laser, synchrotron and optical laser radiation and their users. Under EUCALL, they work together on their common methodologies and research opportunities, and develop tools to sustain this interaction in the future. EUCALL involves 11 partners from nine countries, including major European synchrotron and free electron laser facilities as well as the networks Laserlab-Europe and the Extreme Light Infrastructure (ELI) facilities (https://www.eucall.eu).

The main objectives of Laserlab-Europe are:

- to maintain a competitive, inter-disciplinary network of European national laser laboratories;
- to strengthen the European leading role in laser research through Joint Research Activities (JRA);
- to offer transnational access to top-quality laser research facilities.

Access is offered to research teams from Europe and to a limited extent also to scientists from outside Europe. It is provided:

- to world-class laser research facilities, including two free electron lasers,
- to a large variety of inter-disciplinary research, including life sciences,
- free of charge, including travel and accommodation.

Access is provided on the basis of scientific excellence of the proposal, reviewed by an external and independent Selection Panel. Priority is given to new users. A typical access project has a duration of 2 to 4 weeks.

Details about the submission procedure can be found on the Laserlab-Europe web pages (https://www.laserlab-europe.eu/transnational-access).

Applicants are encouraged to contact any of the facilities directly to obtain additional information and assistance in preparing a proposal. Applications for access are possible anytime. Young researchers and scientists who have never used lasers in their research before are particularly welcome. Laserlab-Europe strives to promote gender equality in scientific research and specifically encourages applications from women.

P-26 **Monday, 04.09., $16^{30} – 19^{00}$**

Physical properties of glass with high manganese content

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Glass with manganese oxide have received much attention because of their importance in technological applications such as catalysts, sensors and new magnetic materials. These materials can also be used in spintronic devices. Especially, manganese silicate, borate and phosphate glasses exhibit unique electrical and magnetic properties, because they can be prepared with a high amount of MnO, even exceeding 50mol%. The content of manganese, their valence states and distribution homogeneity in the glass network depend mainly on the properties of modifiers and glass formers, size of the ions forming glass, their field strength and mobility of the modifier cations. Hence, the relation between physical properties of the host glass and the ionic state and local structure of the manganese atoms is a crucial aspect of the design of materials for special applications.

Manganese silicate glasses exhibit interesting magnetic properties which have been investigated by several authors. It was found that magnetic susceptibility shows Curie-Weiss behavior with a large negative paramagnetic Curie temperature indicating the presence of strong antiferromagnetic exchange interaction [1]. In addition, some anomalous behavior in specific heat was observed [2]. These anomalies can be explained by assuming that glasses contain small (~5nm) regions with antiferromagnetical orientation. However, in the literature, there is a little information about their electrical properties. McMillan [3] shown that when the MnO-Al_2O_3-SiO_2 glasses are submitted to thermal treatment in air at 600°C the surface resistivity decreases about 5 orders of magnitude. This effect can be explained as a result of conversion of a part of the Mn^{2+} ions to Mn^{3+} state.

Manganese in glasses can play a role of glass modifier (with coordination number of six) or network former (with tetrahedral coordination). In silicate glasses Mn^{2+} and Mn^{3+} ions occupy tetrahedral and octahedral sites and the amount of each Mn valence state can be modified by high temperature treatment in oxygen atmosphere. The presence of manganese ions in different valence state and the Mn^{2+}/Mn^{3+} ratio significantly affect the electrical conductivity of these glasses, which can be described by the small polaron hopping between Mn^{2+} and Mn^{3+}. Our experiments have shown that in borate and phosphate glasses submitted to high temperature treatment in oxygen atmosphere the electrical conductivity can also be changed in a controllable way (choosing proper treatment time and temperature). However, electrical properties of manganese borate and phosphate glasses are different from manganese silicate ones. Additionally, the silicate glasses with manganese are less homogeneous and exhibit phase separation in nanoscale. For this reason, regions with high concentration of magnetic ions (monodomains) can be found in these materials.

Differences in electrical conductivity and magnetic properties of manganese glasses with different glass formers can be explained by determining oxidation state, local environment and magnetic moments of manganese ions.

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P-27 **Monday, 04.09., 16^{30} – 19^{00}**

XAFS analysis of niobium-doped bioactive calcium-phosphate glass-ceramics

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Synthetic calcium-phosphate based glasses and glass-ceramics play a crucial role in the development of tissue engineering. These materials have a high biocompatibility with biological analogues, excellent ability to undergo varying degrees of resorbability [1] and due to their non-toxicity and relatively high bioactivity they are commonly used as bone and dental implants. A substantial research effort is devoted to improve synthetic calcium-phosphate materials physico-chemical properties, inter alia tune the degree of crystallinity which is mainly responsible for material solubility. One of the strategies is their doping with metal ions. The results found in the literature show that synthesized CaO-P_2O_5-Nb_2O_5 compounds exhibit a good biocompatibility, very low cytotoxicity in respect to calcium-phosphate doped with other metals and additionally can enhance human osteoblast function [2]. Moreover, a really few information on the structure of these materials can be found in the literature and no detailed structural analysis which can shed light on the relationship between structural parameters and dopant contents, preparation technique or sample porosity. Therefore, during measurements realized at ELETTRA (XAFS beamline) the spectra in XANES and EXAFS (up to 800 eV above the absorption edge) ranges were collected at Nb K-edge (18986 eV) at RT using a transmission geometry for a set of CaO-P_2O_5-Nb_2O_5samples with different Ca/(P+Nb) molar ratio and different relative amount of Nb ions, prepared by melt-quenching (MQ) method (as prepared and annealed at 800°C and 900°C) and sol-gel (SG) method. Pre-edge background linear subtraction and normalization of the X-ray absorption spectra were carried out to facilitate a qualitative comparison between subsequent measurements. To obtain a detailed structural information about local niobium environment in the samples and its correlation with sample stoichiometry and preparation technique, EXAFS data were analysed using the GNXAS software package [3,4]. Spectra of reference samples (niobium dioxide and pentoxide) were also analysed to construct proper model for data elaboration.

In this work, we show only the results obtained for bioactive glass-ceramics with Ca/(P+Nb) molar ratio equal to 1.0. Figure 1 presents Nb K-edge normalized XANES spectra of the samples prepared by melt-quenching (left panel) and sol-gel (right panel) methods as a function of relative Nb contents (from 0 to 10 mol% of P ions). The reference samples are also included for comparison. It should be emphasized that XAFS spectra of all samples are identical, independently on the synthesis method and Nb contents. Detailed EXAFS analysis show that in all samples octahedral coordination of niobium ions dominates (like in niobium pentoxide). This result is confirmed by XPS analysis, which showed that the contribution of Nb^{+5} in respect to Nb^{+4} is about ten times greater. At the same time, a huge differences are observed as regard the sample morphology and porosity (SEM imaging results). Moreover, decreasing absolute Nb amount leads to the more ordered Nb local structure. Subtle changes in niobium oxide subnetwork continuity has also been detected as a function of materials stoichiometry.

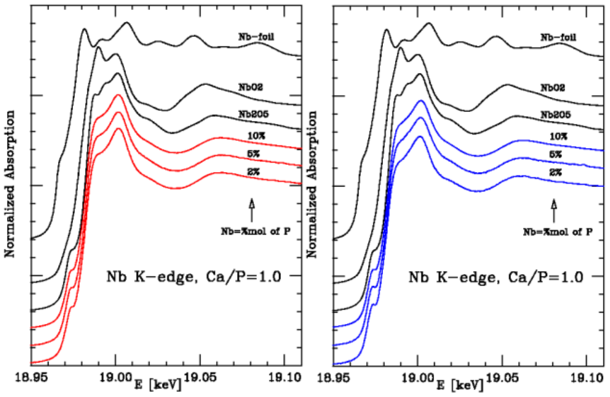

Figure 1. XANES of samples prepared by MQ and SG methods.

Acknowledgements: We gratefully acknowledge the support of the SLL ELETTRA in providing synchrotron radiation facilities (XASF11.1 station) for 20160241 experiment.

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P-28 **Monday, 04.09., 16^{30} – 19^{00}**

Systems based on trimetric surfactants and lipids as nonviral vector for gene therapy

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The ability of cationic surfactants to bind nucleic acid makes them one of the potential non-viral vectors for gene therapy. Effective transfection process – the transport of the genetic material into the cells – is the main challenge of modern, innovative therapies. Nanosystems based on selected trimeric surfactants and phospholipids (phosphatidylcholine derivatives) have a great potential to become effective vectors for gene therapy [1-4]. Such mixed systems, i.e surfactant with naturally occurring in membranes lipids, represent a compromise between the biocompatibility provided by lipid molecules and toxicity of surfactants, which presence is necessary due to their binding ability that ensures the effectiveness of complexation of nucleic acids [1-4].

First step of our studies is to estimate the ability to bind nucleic acids and select mixed systems that are characterized by high capability of binding DNA but also to release it from the complex (electrophoretic testes). We focus on three trimeric surfactants, several lipids (such as DMPC, DOPE, DPPC) and DNA varying in size i.e. 21 bp, 200 bp and 20 kbp. Next step is to obtain structural information about formed systems (small angle X-ray scattering SAXS), characterize conformational changes within the lipid structures and investigate the nature of phase transitions in solution (infrared spectroscopy FTIR, differential scanning calorimetry DSC).

Trimeric surfactants complexed with DNA more effectively than theirs monomeric forms due to multiplied positive charges. Addition of lipids also improves the efficiency of the complexation and thus lower the concentration of surfactants that is necessary to form complex and therefore the toxicity of such vector decreases. Studied surfactants built into the lipid bilayers, forming domains and changing its flexibility – bilayer becomes more fluid. They also induce the formation of unilamellar structures as the lamellar structures were formed in lipids solutions without surfactant addition.

Acknowledgements: This work was supported by grant from National Science Centre (Poland), Project No. 2014/15/N/ST5/02003.

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P-29 **Monday, 04.09., $16^{30} – 19^{00}$**

Photoisomerisation of *nitro* group in crystals of transition metal complexes - home laboratory vs. synchrotron studies

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Currently, one of main goals of chemistry and physics is to develop new materials that are able to respond rapidly and reliably to changes in local environment, and send out signals that let us know what is happening. Transition metal switchable complexes, thanks to the specific interactions and presence of the groups that can exist in many isomeric forms, as well as, their interesting optoelectronic and magnetic properties, very often fulfil these criteria. The unique properties of such complexes have important consequences in both materials science and biology.

Hence, this contribution is devoted to photocrystallographic studies of NO_2-isomerisation in crystals of nickel(II) nitro complexes. Depending on the sample properties (*e.g.* diffraction quality, metastable state lifetime) and laboratory capabilities, such experiments can either be performed at synchrotron sources, or at home laboratory. We will describe home measurements using the light-delivery device designed by us for *in situ* photocrystallographic experiments [1] and present literature examples of synchrotron studies of this kind, giving the advantages/disadvantages of both solutions.

We will focus on three cases, which all are nickel complexes. The first example is the $Ni(dppe)(NO_2)Cl$ complex which has initially been reported by Warren *et al.* [2], and also studied by us employing our light delivery device. The crystal undergoes nitro group isomerisation when irradiated with 400 nm LED diode. After about 60 minutes full conversion is reached. In turn, the second complex is a half sandwich compound coordinated additionally with the N-heterocyclic carbine (NHC) and nitro ligands. This system constitutes a nitro derivative of a known nitrate polymerisation or cross-coupling reaction precatalyst. [3] Our preliminary studies have shown that the molecule of this compound switches from the nitro to nitrito form upon irradiation with 470 nm LED light. After 1.5 h of the crystal irradiation at 100 K the system becomes a mixture of both forms. Whereas at temperatures higher than 150 K the metastable nitrito state converts back to the parent nitro form. Finally, the third, literature example shows the potential of synchrotron experiments in studies of metastable species. The $Ni(PCy_3)_2(NO_2)_2$ complex linkage isomerism was here investigated by Warren *et al.* After crystal irradiation with 400 nm wavelength at 100 K three different orientations of the NO_2 ligands were observed in its structure. The components consisted of the nitro ground state species, an endo-nitrito (ONO) species and an exo-nitrito to ONO species with determined occupancies equal to 18, 62, and 20% respectively.[4] In general, synchrotron sources are indispensable in metastable states' studies, especially when crystals are small and weakly diffracting. Small crystal sizes assure better light penetration of the crystal volume. Also, synchrotron experiments are much faster.

Such studies are important considering materials science, new technologies and innovations. The desired photoswitchable materials should be characterised by full conversions (100%), controllable reversibility, stability and preferably switching observable at temperatures closest to room temperature.

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P-30 **Monday, 04.09., 16^{30} – 19^{00}**

ARPES and STM/STS data correlation in investigations of doped graphene on 4H-SiC(0001) and Ge(001) surfaces

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Graphene is a material that has unique properties allowing for the movement of charge carriers without backscattering due to conservation of pseudospin quantity. Even though mobility of carries is extremely high for this material the electrical conductance is not satisfying. This is caused by the small number of carries close to the Fermi level in unperturbed graphene. The very effective method to increase the number of carriers is doping process induced by graphene/substrate interaction or incorporation of foreign atoms during the graphene synthesis process.

We show our studies related to doping process of graphene/4H-SiC(0001) samples by hydrogen intercalation and nitrogenation. Interaction between graphene and Ge(001) substrate is also discussed. Especially, we focus on correlation of *E(k)* data obtained by the ARPES technique with local density of states function *LDOS(x, y, E)* collected by STS/CITS methods. The obtained results are discussed in the frame of DFT calculations performed using QUANTUM ESPRESSO package. The representative set of STM/STS/ARPES data collected for graphene/4H-SiC(0001) doped by nitrogen is presented in *Fig.1*.

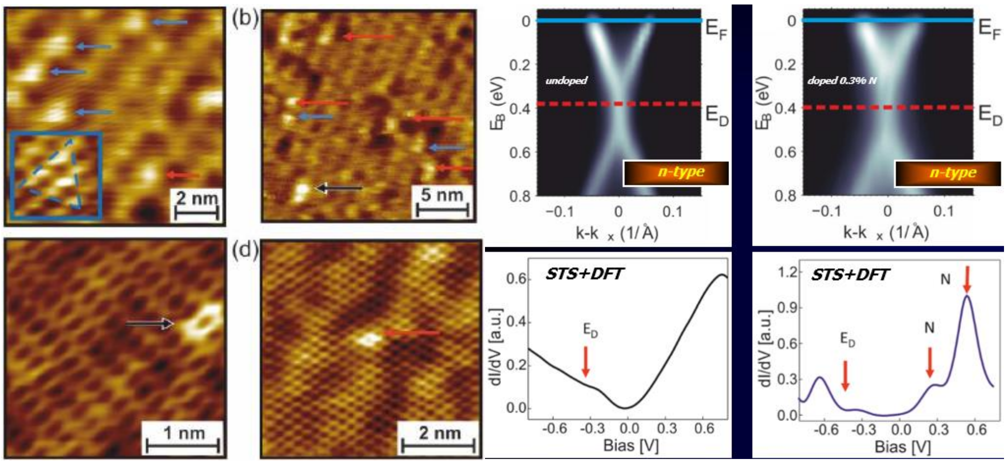

Figure 1. STM/STS and ARPES results collected for nitrogen doped graphene/4H-SiC(0001) sample.

Acknowledgement: The work is financially supported by The National Science Centre, Poland (research grant No. 2015/19/B/ST3/03142).

P-31 **Monday, 04.09., 16^{30} – 19^{00}**

Investigation of selected gold nanoparticle and nanoribbon systems using SAXS, AFM and spectroscopic techniques

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Gold nanoribbons (GNr) belong to a novel subgroup of gold nanoparticles family (GNp) and exhibit unique properties, resulting from their ribbon-like morphology, which can be utilized in various fields of science, from nanotechnology to nanomedicine. The goal of our research was to optimize the synthesis of GNr's and develop applications of these nanosystems as components of nanosystems used for drug delivery or in nanosensing.

In this presentation we would like to show first step of our work, which is focused on the optimal way of GNr's synthesis using GNp and dimeric surfactants and characterization of GNr morphology. We used the small angle X-ray scattering (SAXS) method for the investigation of structural parameters of various types of the nanoparticles obtained. Also we would like to compare SAXS data with structural information (sizes and shapes of gold nanoparticles) obtained, using the atomic force microscopy (AFM). The modification of surface of studied nanoparticles by surfactant molecules and intermolecular interactions between GNr's and surfactants, confirmed by the FTIR spectroscopy, will be also presented.

P-32 **Monday, 04.09., 16^{30} – 19^{00}**

Phosphorylated prion peptide PrP$^{40\text{-}49}$ unfolds WW domain of PIN1 peptidyl-prolyl *cis-trans* isomerase

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Human prion protein (huPrP) is a membrane glycoprotein (253 amino acids, 28 kDa, glycophospatidylinositol anchor), produced at high levels in brain neuronal cells [1]. Structural studies (NMR, X-ray crystallography) allowed characterization of PrP structure, which in the native state (cellular form denoted as huPrP^{C}) consist of unstructured N-terminal domain and ordered predominantly α-helical C-terminal domain [2-4]. Under certain conditions PrP^{C} (pH, denaturing conditions or presence of misfolded, pathological PrP molecules) can undergo a structural transition into insoluble, β-sheet rich and form (denoted as PrP^{Sc}) [4,5].

Other physiologically important protein is PIN1. This is peptidyl-prolyl isomerase (PPI) that perform *cis-trans* isomerization of phosphorylated S/T-Pro peptide bond. In huPrP only one possibility namely Ser43 – Pro44. As shown previously, the phosphorylation Ser43 lead to structure alterations [6,7]. We postulate, that phosphorylated substrate interacted with PIN1 resulted in speed-up process of PrP^{C} → PrP^{Sc} transformation.

The goal of our studies was to check if phosphorylated peptide (PrP$^{40\text{-}49}$) based on human prion protein sequence can interact with PIN1 and alter its structure and function. Therefore, we performed Small Angle X-ray Scattering studies of PIN1-PrP$^{40\text{-}49}$ systems. Experimental SAXS data were used for modelling of low resolution structure in solution using the EOM procedure [7]. The results obtained indicate, that pPrP$^{40\text{-}49}$ is able to unfold WW domain of a PIN1 protein, which makes *cis-trans* isomerization inefficient *in vitro*.

Acknowledgements: This work was supported by National Science Centre, Poland, under grant No. 2014/15/B/ST4/04839.

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P-33 **Monday, 04.09., $16^{30} - 19^{00}$**

High pressure studies on racemic and enantiopure 1-benzoyl-3-(1-phenylethyl)thiourea

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Most of the biologically active substances are chiral and enantiomers can interact differently with living organisms. Hence, enantiomer resolution and asymmetric synthesis are of great importance for the pharmaceutical, chemical, and food industries.

In 2013 we have reported our X-ray diffraction studies on racemic 1-benzoyl-3-(1-phenylethyl)thiourea (**1**) and its *S*-enantiomer (**2**) [1]. In next two years both *R* and *S*-enantiomers of this ligand were successfully used in synthesis of chiral ruthenium(II) catalysts for stereoselective reduction of ketones [2,3].

On the other hand, chiral resolution can be done chromatographically or, sometimes, by crystallization. According to Wallach's rule [4,5], racemates form denser, more stable crystals than enantiomers. However, the validity of the rule is often broken and many exceptions have been reported so far [6].

High pressure favours high density solids and therefore can be applied for enantiomeric resolution of the chiral compounds defying Wallach's rule [7]. It has been estimated by Jacques, Collet, and Wilen that the racemates less dense than the enantiomers should be spontaneously separated below 1 GPa [8].

Here we report our high pressure study of **1** (monoclinic crystals, space group $C2/c$) and **2** (orthorhombic crystals, space group $P2_12_12_1$) up to at least 3.45 GPa. A series of high-pressure single-crystal diffraction experiments have been performed at High Pressure ID09A Beamline at ESRF (Grenoble, France) using parallel monochromatic X-ray beam (E = 30 keV, λ = 0.413 Å) focused to 30 × 30 μm on the sample loaded into membrane Diamond Anvil Cell and topped by silicon oil.

Similarities and differences in **1** and **2**, as well as potential possibility of resolution under high-pressure will be discussed within the poster.

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National Synchrotron Radiation Centre SOLARIS - current status and future development

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SOLARIS - National Synchrotron Radiation Centre in Kraków is the most modern and largest multidisciplinary research facility in Poland. The Centre was built in remarkably short time - only five years from the signing in 2010 the agreement between the Ministry of Science and Higher Education and Jagiellonian University. The investment was co-financed by the European Union with funds from the European Regional Development Fund, as part of the Innovative Economy Operational Programme.

SOLARIS utilizes the groundbreaking design of magnetic double bend achromats developed at MAX-lab facility in Lund, Sweden, resulting in outstanding properties of generated synchrotron light which places SOLARIS firmly at the cutting edge of devices of this type. SOLARIS synchrotron operates at 1.5GeV energy with up to 500mA stored electron beam. It is powered by 600MeV S-band linac.

SOLARIS can provide synchrotron radiation for up to 18 beamlines from bending magnets and insertion devices. Within the scope of the project budget already two experimental beamlines have been constructed.

Since completion of the project (Dec 2015) the SOLARIS team has been focused on commissioning of the linac, storage ring and the two beamlines. Even with a very broad help from our colleagues from synchrotron facilities abroad it has been an immense challenge. As usually, such a new - and in the SOLARIS case - unique infrastructure, requires fine tuning and optimization. This include many aspects such as machine optimization, alignment corrections, control system improvement, temperature stabilization, to name the few. Today, for quite a while, SOLARIS synchrotron operates with regular few hundreds of mA two times per day filling scheme. The target of 500 mA has also been routinely achieved.

Two experimental beamlines equipped with three end stations are about to start operation.

Photoemission Electron Microscopy / X-ray Absorption Spectroscopy (PEEM/XAS) - the bending magnet beamline is dedicated to microscopy and absorption spectroscopy research in the range of soft X-rays (200-2000eV). PEEM/XAS beamline has been built in collaboration with Institute of Catalysis and Surface Chemistry PAS, and Academic Centre for Materials and Nanotechnology at University of Science and Technology in Kraków and will be ready for the first measurements for the first light in autumn, after the summer Solaris shut down.

The Ultra Angle-Resolved Photoelectron Spectroscopy (UARPES) beamline constructed in collaboration with Jagiellonian University Institute of Physics is an undulator beamline offering angle resolved study of photoelectron emission in the 8-100eV range of photons energy. The beamline already experienced friendly users operation, however, due to some mechanical and outgassing problems of the motorized monochromator manipulators, that activity had to be suspended for few months and some components sent for the correcting action to the manufacturer.

Figure 1. Inside SOLARIS storage ring tunnel: double bend integrated achromats and UARPES beamline undulator.

It is expected that during the 2017 fall both beamlines will host the so called friendly users groups whose expertise will help and speed up the process of fine tuning and calibration of the beamlines.

SOLARIS comprehensive offer for the research and industrial community will be only possible with the further funding allowing for building the full set of the beamlines offering broad spectrum of experimental techniques. 2017 has been so far very successful in this field.

Funds for building two next beamlines have been granted:

The PHELIX beamline is aimed to perform studies of the electronic structure of solids with high energy - resolution, using soft X-rays in 50-1500eV range with variable polarization. It will be equipped with ARPES end station. Institute of Physics of Silesian University is involved in the project.

The tender for construction of the beamline has been just recently concluded and the work on the detailed design has already started. The beamline should be in operation in the three year time.

The XMCD is a soft X-ray beamline, covering the energy range 200 to 2000 eV of photons from an elliptically polarizing undulator, providing linearly and circularly polarized radiation. It is intended for study of magnetic circular dichroism (MCD). This beamline has been transferred from Sweden due to the agreement between SOLARIS and MAX IV laboratory as a result of a strong initiative and participation of many Polish groups and University of Uppsala. The funds will allow for refurbishment and reinstallation of the beamline at SOLARIS. The project is currently taking off starting with tendering process.

Moreover, there is a firm prospect for funding the construction of the high energy, wiggler based, MX-SAXS-PD beamline allowing for material and structural studies with high energy photons. Such a beamline has been eagerly expected by many Polish research groups and industry. The conceptual design is being developed in collaboration with Adam Mickiewicz University in Poznań.

Additionally, two applications are being prepared for funding: an FTIR microspectroscopy beamline (operating in the IR region) and high energy (2-10keV) bending magnet beamline offering XANES (X-ray Near Edge Absorption Spectroscopy), EXAFS (Extended X-ray Absorption Fine Structure Spectroscopy) and XES (X-ray Emission Spectroscopy) techniques. The latter being initiative of the Institute of Physics of Polish Academy of Sciences.

More detailed information on all the above actions and even further plans will be given by SOLARIS team members during the KSUPS'17 separate sessions, in the proceedings, and are available at www.synchrotron.pl

Our Digital Users Office will be available in the autumn for submission of the proposals. Its test launch is planned during KSUPS'17.

From the January 2018 SOLARIS team is eagerly awaiting the first regular users.

To conclude, the participation of SOLARIS in Central European Research Consortium CERIC – ERIC should be mentioned, where seven central European countries agreed to offer free access to their delegated research facilities with comprehensive technical and scientific support. This opens unique opportunities to Polish researchers. More information can be found at www.ceric-eric.eu.

Polish Researchers in European Synchrotron Radiation Facility

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The scientific tools nowadays are very expensive and the improvement in technology and electronics is so quick that even very rich countries cannot afford the cost of continuous upgrading. As the synchrotron users perfectly know, the only economic solution is the creation of international laboratories used by wide community of scientists. The good examples are synchrotrons, particularly the European Synchrotron Radiation Facility in Grenoble, France (ESRF- www.esrf.eu). In 1988, eleven European countries joined forces to build this world's most performing and bright facility, dedicated to production of light. Today, 22 countries operate and finance it jointly. On 19 June 2017 the India joined with 0.66% contribution. Almost thirty years after creation this visionary project has made an outstanding contribution to the excellence of European science.

Figure 1. ESRF in Grenoble (with ESRF permission).

On 20th December 2016, in the Institute of Physics, Polish Academy of Science (IP PAS) the signature of the Arrangement between IP PAS and ESRF took place. The arrangement is concerning the long-term scientific use of the synchrotron radiation by Polish scientists. IP PAS was represented by the Director Prof. Roman Puzniak, ESRF - by General Director Dr Francesco Sette. In the ceremony participated the IP PAS scientific director Dr Tomasz Sowinski, secretary of the ESRF council Itziar Echeverria, Prof. Krystyna Jablonska, who is from very beginning representing Poland in the ESRF Council. Furthermore, 16 from 20 of the representatives of the Consortium of the scientific institutions in Poland interested in use of this best in the Europe high energy synchrotron, were present. IP PAS acts as a coordinator of this Consortium. The signature of Arrangement was possible after the decision made on 6th December 2016 by the Minister of Science and Higher Education Jaroslaw Gowin for allocation of the financial resources to pay the Polish contribution at the level of 1% of ESRF yearly budget. The decision secures the access of Polish scientists to this world's most intense X-ray source for five years (till March 2021). Each scientist with Polish affiliation can propose experiment at 43 beamlines with modern equipment related to x-ray techniques. After positive evaluation by the international scientific committee the time for measurements is allocated and the travel and accommodation for three scientists participated in experiments is paid by the facility. Synchrotron is operating 7 days per week, day and night. Poland is an associated member of ESRF from May 2004. It was the result of 10 years continuous efforts of the Polish scientists gathered in the Polish Synchrotron Radiation Society (PTPS-www.synchrotron.org.pl). Polish researchers fully explore the scientific power of this facility. More than 50 papers are published each year from the results of experiments performed there by Polish scientists. They used 1% of the beamtime available at all experimental stations at ESRF. More information at - http://www.ifpan.edu.pl/esrf/Local_Publish/.

Figure 2. (left) After signature at IP PAS of Arrangement in 2016. From left: R. Puzniak, K. Jablonska, F. Sette (photo by W. Paszkowicz).

Figure 3. (right) After signature at ESRF of Arrangement in 2004, by Director IP PAS J. Kossut (in the middle), Director General ESRF B. Stirling (on right) and Helmut Krech (on left), the ESRF Director of the Administration (photo by K. Jablonska).

A-03 **News from the ESRF**

The future is always bright!

Interview with Dr. Francesco Sette, Director General ESRF

(Dec 20, 2016, interviewer: Wojciech Paszkowicz)

Could you please comment the comeback of Poland to the ESRF?

Can I say something true? Poland has never left the ESRF...

You are right.

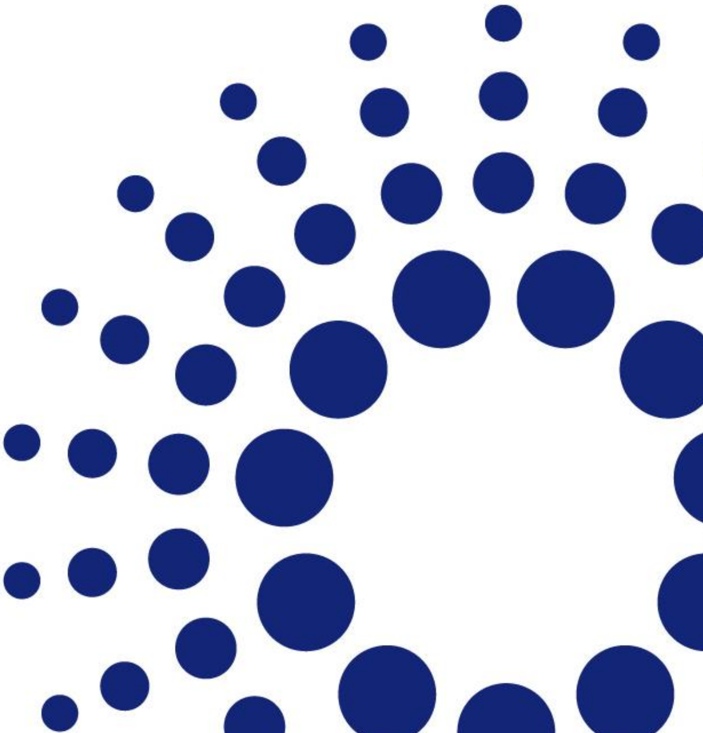
The ESRF Council was extremely understanding of some financial difficulties. We always recognized the importance and quality of Polish work at the ESRF. So I just want to underline that today we solved an important issue and I am extremely pleased to also recognize the strong support of the Ministry of Science in our collaboration. But I never had a doubt that the ESRF will continue to exist without a contribution from Polish scientists.

What about the activity of prof. Krystyna Jablonska, aiming for maintaining the membership of Poland in ESRF?

The activity of Krystyna Jablonska was absolutely fundamental during these many years. Krystyna knows the ESRF extremely well. She has been doing research at the ESRF, she has been representing Poland for many years in the ESRF council, and without her it would be impossible to renew this collaboration on long term basis... So without her it would be impossible to really put together all the elements necessary for finalizing the signature of arrangement. So I am very grateful for her and I am convinced that when she will come back to ESRF and maybe to continue to represent Poland at the ESRF Council, the next Council meeting in June 2017, we will be extremely pleased to thank her globally.

Is the future bright for us?

The future is always bright!



The high pressure crystallography beamline ID15B of the ESRF

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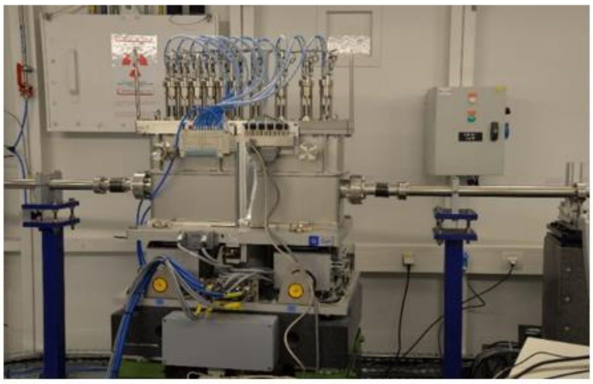
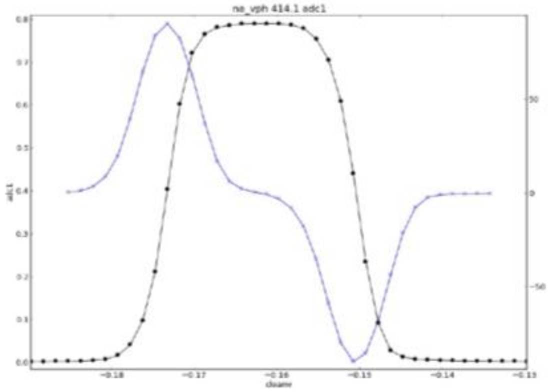
ID09A [1] was a state of the art high pressure diffraction beamline at the ESRF, carrying out monochromatic diffraction experiments with large area detectors. Powder and single crystal diffraction experiments could be performed at high pressures in diamond anvil cells, permitting accurate determination of crystallographic properties of the investigated samples. After more than 20 years of successful operation, ID09A has been closed in November 2015. It has been replaced by a new and vastly improved beamline, ID15B, which started operation in November 2016.

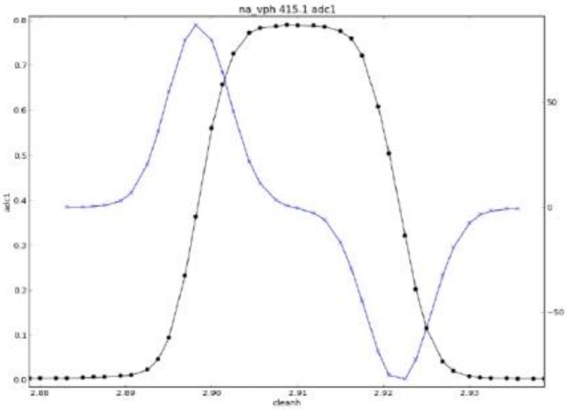
On ID15 two beamlines with a canted straight section have been constructed. The first one (ID15A) is for materials chemistry and engineering applications, the second one (ID15B) for monochromatic high pressure diffraction with large area detectors, replacing ID09A. Due to canting the two beamlines can be operated independently.

X-ray source for ID15B is the U20 in vacuum undulator from ID09A. The monochromator is a horizontally diffracting nitrogen cooled Si (111) single bounce Bragg monochromator. ID15B operates at a fixed angle with an energy of 30 keV. Experience with ID09A has shown, that 30 keV is well matched for high pressure diffraction experiments in DACs. Two transfocators (Fig. 1) with 200 μm diameter linear (1-D) beryllium compound refractive lenses for vertical and horizontal focusing, respectively, provide a highly variable and very clean beam with a minimum spot size on the sample of less than 7 x 7 μm^2.





vertical



horizontal

Figure 1. Horizontal transfocator and beam through a 20 μm pinhole.

The flux is comparable to ID09A. The experimental setup, build mostly from components already in use on ID09A, is located on an extremely stable granite table. Data are collected with the MAR555 flat panel detector. The ID09A sample preparation and Laser laboratory have been relocated to accommodations close to the beamline.

ID15B offers similar possibilities for data collection as ID09A, powder and single crystal diffraction with high resolution well into the megabar pressure range, with, if requested, variable temperatures from a few to several hundred Kelvin. An example of a single crystal data collection is given in Fig. 2.

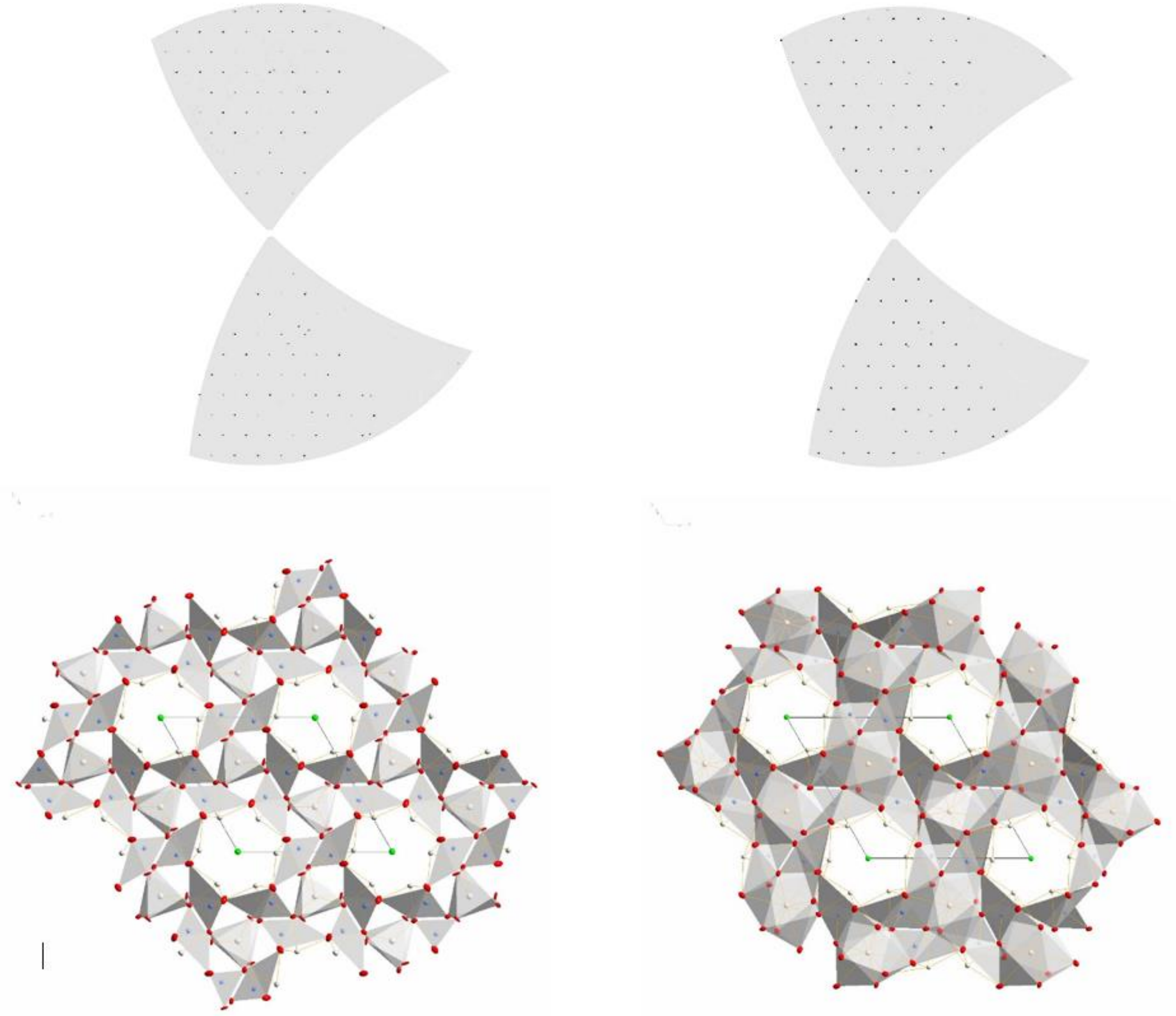


Figure 2. Reciprocal space reconstruction and refined structure of Vanadinite, $Pb_5(VO_4)_3Cl$, S.G.:P63/m, at 0.16 and 18.4 GPa, respectively. Vanadinite belongs to the Apatite family of minerals. It can be considered as a framework of Pb - O and V – O polyhedral with the Cl – atoms in the center of hexagonal channels. With increasing pressure the framework becomes noticeably more compact, while the channels remain essentially unaffected.

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[1] M. Merlini, M. Hanfland, *Single-crystal diffraction at megabar conditions by synchrotron radiation*, High Pressure Research **33** (2013) 511.

News

Synchrotron Light News

First ARPES maps from SOLARIS

On June 11, 2016, for a first time, a typical experiment for which the UARPES beamline had been designed – the massively parallel angle-resolved photoelectron spectroscopy experiment – was performed. An electronic structure around Dirac point were measured on graphene.

New beamlines soon at SOLARIS

On June 30, 2017, an agreement for design, construction and assembly of PHELIX beamline has been signed with FMB Feinwerk- und Messtechnik GmbH. The PHELIX beamline is designed to perform studies of the electronic structure of solids with high energy - resolution, using soft X-rays with variable polarization providing radiation in the energy range 50 - 1500 eV. The main technique will be photoelectron spectroscopy including an angle resolved option. The layout of the beamline allows using the light from the same source also for soft X-ray spectroscopy studies.

Recently, the Ministry of Science and Higher Education, Poland, has granted founds for the refurbishment and retrofit programme of the elements of I1011 beamline imported from MaxLAB II as well as their assembly as XMCD beamline.

Open SESAME

After achiving a first beam of circulating electrons on January 11, 2017, the International Centre for Synchrotron-Light for Experimental Science and Applications in the Middle East has been officially inaugurated on May 16. SESAME was set up on the model of CERN and construction work on the $100 million centre started in 2003 in Jordan. It was further developed under the auspices of UNESCO. SESAME's Members are Bahrain, Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, the Palestinian Authority and Turkey. Its mission is to provide a world-class research facility for the region, while fostering international scientific cooperation. The centre also has 17 observers, who have an advisory role and include the European Union, China and the United States.

TPS operational

On September 19, 2016, the Taiwan Photon Source (TPS) synchrotron has been inaugurated. It hosts a 3GeV storage ring and seven beamlines constructed within the Phase I of the TPS Experimental Facility Construction Project.

SwissFEL Inauguration

On December 5, 2016, the Paul Scherrer Institute (PSI) held an inauguration ceremony for its new large-scale research facility SwissFEL. The costs of SwissFEL amount to around 275 million Swiss francs and were largely borne by the federal government. Canton Aargau was also participating in the financing with 30 million francs out of its Swiss Lottery funds. The first pilot experiments at ARAMIS hard X-ray beamline have started in 2017.

First beam in the European XFEL experimental hall

On June 23, 2017, a first successful guiding of the X-ray laser beam to reach the SPB/SFX and FXE optics hutches of the European XFEL was achieved. It was an important milestone in the preparation for the start of user operation in September his year. In May, DESY and European XFEL successfully produced the first laser light in the tunnel. After several weeks of further progress, the laser beam has now reached the experiment hall in Schenefeld.

New experimental hall of Petra III

On September 14, 2016, the research centre DESY held an inaugural ceremony celebrating two new experimental halls at the X-ray lightsource PETRA III named after Nobel Prize laureate Ada Yonath and Paul P. Ewald. These halls can house up to five additional PETRA III beamlines each, expanding the range of research that can be carried out at PETRA III. Three of the beamlines in PETRA III's new experimental hall "Ada Yonath" were built in collaboration with scientists from India, Sweden and Russia.

Four new beamlines at ESRF

On June 27, 2017, the ESRF Council gave the green light for the construction and commissioning of four new beamlines from 2018-2022. The beamlines are designed to exploit the enhanced performance of the first of a new generation of synchrotron, the Extremely Brilliant source (EBS), which is being built at the ESRF. These beamlines will serve for: Serial Macromolecular Crystallography, Hard X-ray Diffraction Microscopy, Coherent X-rays Dynamics and Imaging Applications, and High Throughput Large Field Phase-contrast.

Gersh Budker Prize 2017

Dr. Pantaleo Raimondi, ESRF's Accelerator & Source Director, received the 2017 Gersh Budker Prize of the European Physical Society Accelerator Group for his "invention of the Hybrid Multi Bend Achromat (HMBA) lattice", "which has become the design basis of most future 4th generation synchrotron sources". The Prize was awarded on May 18, during the International Particle Accelerator Conference, IPAC'17, in Copenhagen.

Gregori Aminoff Prize 2017

The Royal Swedish Academy of Sciences has awarded the Gregori Aminoff Prize in Crystallography 2017 to Professor Natalia Dubrovinskaia and Professor Leonid Dubrovinsky of University of Bayreuth, Germany "for having developed new methodology for in situ-experimental determination of crystal structures subjected to extreme conditions of high temperature and pressure". The Prize Ceremony was held during the Royal Swedish Academy of Sciences' annual celebration on March 31.

ESRF Young Scientist of the Year 2017

The Young Scientist Award was presented to Amélie Juhin for her experimental and theoretical studies of resonant X-ray scattering and X-ray dichroism. The prize was announced during the 27th ESRF annual User Meeting in Grenoble, on February 7.

ACA Prizes 2017

The American Crystallographic Association has presented four awards during May 26-30 meeting held in New Orleans. Patterson Award was presented to Zbigniew Dauter from Advanced Photon Source, David Rognlie Award to Helen M. Berman from The State University of New Jersey, Elizabeth Wood Science Writing Award to James O'Brien from Missouri State University, and Etter Early Career Award to Christine Dunham from Emory University School of Medicine.

Innovation Award on Synchrotron Radiation 2016

The 2016 Innovation Award on Synchrotron Radiation been given on December 8, in Berlin-Adlershof to Dr. Christian Tusche from Forschungszentrum Jülich for his pioneering paper on “Imaging Spin-Filters for Spin-Resolving Momentum Microscopy”. Working at the Max Planck Institute of Microstructure Physics, Halle/Saale, and BESSY II he has showed that the efficiency of spin-resolved electron spectroscopy can be increased by up to four orders of magnitude. The Innovation Award on Synchrotron Radiation is sponsored by SPECS GmbH and BESTEC GmbH.

Ernst Eckhard Koch Prize 2016

The Association of Friends of Helmholtz-Zentrum Berlin awarded the 2016 Ernst Eckhard Koch Prize to Dr. Jan Wernecke for his doctoral dissertation “When Size Does Matter: Dimensional Metrology of Nanostructured Layers and Surfaces Using X-Rays” at the Technische Universität Berlin. He employed small-angle X-ray scattering for measuring nano-dimensional features on surfaces and thus established standard metrological data traceable back to the international system of units SI with uncertainties in the range of a few atomic diameters.

Schieber Award 2016

The 2016 Schieber Award for excellent ground-breaking work to date, as well as for the promise for future contributions to crystal growth science and technology was awarded at the 2016 International Conference on Crystal Growth in Nagoya, to Dr. Alexander van Driessche from ISTerre, CNRS and University Grenoble. The Prize of International Organization for Crystal Growth is sponsored by the Journal of Crystal Growth.

Science@FEL Prize 2016

During the Science@FELs conference held in September 2016 in Trieste, the "FEL Science and Applications" prize has been awarded to Dr. Kartik Ayyer, a young scientist from the Center for Free Electron Laser Science (CFEL), a joint enterprise of DESY, the Max Planck Society (MPG), and the University of Hamburg, for his novel methodology developed for macromolecular diffractive imaging using imperfect crystals.

Microscopy Today Award 2016

Scientists working at NSLS-II are proud recipients of one of the 2016 Microscopy Today Innovation Awards, which highlight the 10 best microscopy innovations each year. The award was presented for the development of the Hard X-ray Nanoprobe (HXN) beamline equipped with novel nanofocusing optics based on multilayer Laue lenses (MLL), which produce a tiny x-ray beam of 12 by 13 nanometer spatial resolution. They received the award on July 27, at the Microscopy & Microanalysis 2016 meeting in Columbus, Ohio.

Carousel – synchrotron free time watching, listening and reading

24 hours at the X-ray factory

Nature **531**(7596) (2016) 564.

Reportage from visiting the ESRF synchrotron. *Nature* spent a day and a night at the European Synchrotron Radiation Facility to reveal the science that never sleeps.

- www.youtube.com/watch?v=UsJ1j4_1Di0

UNESCO and SEZAME

Professor Michał Nałęcz, an former member of the SESAME Council UNESCO, explains the role of the centre in the middle-east, recalls the milestones and reveals several not a-well-known stories regarding the project during interviews at Polish Radio 1 and TOK FM (*in Polish*):

- http://audycje.tokfm.pl/gosc/Maciej-Nalecz/4768
- http://www.polskieradio.pl/7/5098/Artykul/1727845,Sesame-jak-CERN-zjednoczy-podzielony-Bliski-Wschod

X-Ray Absorption and X-Ray Emission Spectroscopy: Theory and Applications

J. A. van Bokhoven, C. Lamberti (Eds.) (*Wiley, 2016*)

Two-volume book features articles that explain the phenomena and describe examples of X–ray absorption and emission applications in chemistry, biochemistry, catalysis, amorphous and liquid systems, and surface science.

Hard X-ray Photoelectron Spectroscopy (HAXPES)

J. C. Woicik (Ed.) (*Springer, 2016*)

The first complete summary of the state of the art in HAXPES. Historical works, modern instrumentation, theory and applications, from physics to chemistry and materials science and engineering.

Relativistic Coupled Cluster Calculations with Variational Quantum Electrodynamics Resolve the Discrepancy between Experiment and Theory Concerning the Electron Affinity and Ionization Potential of Gold

L. F. Pašteka, E. Eliav, A. Borschevsky, U. Kaldor, and P. Schwerdtfeger,

Physical Review Letters **118** (2017) 023002.

A long-standing inconsistency between experiments and theory concerning the electronic properties of gold has been resolved when electron correlations calculations were extended to quadruple and pentuple interactions. By doing so, the discrepancy between the ionization energy and electron affinity were reduced to few milli-electron-volts only.

The first direct evidence of a Late Devonian coelacanth fish feeding on conodont animals
M. Zatoń, K. Broda, M. Qvarnström, G. Niedźwiedzki, P. E. Ahlberg,
The Science of Nature **104** (2017) 26.
Using a combined experimental approach including the synchrotron tomography the authors advanced synchrotron he authors study the remains of a Devonian coelacanth from the lower Famennian of the Holy Cross Mountains, Poland. The investigation is a step towards understanding the feeding way of the animal.

Terahertz and mid-infrared plasmons in three-dimensional nanoporous graphene
F. D'Apuzzo, A.R. Piacenti, F. Giorgianni, M. Autore, M. Cestelli Guidi, A. Marcelli, U. Schade, Y. Ito, M. Chen, and S. Lupi,
Nature communications **8** (2017) 14885.
Strong plasmonic absorptions can be tuned via controllable doping level and porosity by the presence of intrinsic 2D Dirac plasmons in 3D nanoporous grapheme opening the way for novel and competitive nanoporous-graphene based plasmonic-sensors.

The pyrite-type high-pressure form of FeOOH
M. Nishi, Y. Kuwayama, J. Tsuchiya, T. Tsuchiya,
Nature **547** (2017) 205.
The formation of a new FeOOH phase with the pyrite-type framework of FeO_6 octahedra, which is much denser than the surrounding mantle has been proposed based on first-principles calculations and in situ X-ray diffraction experiments. Pyrite-type FeOOH may stabilize as a solid solution with other hydrous minerals in deeply subducted slabs.

A public database of macromolecular diffraction experiments
M. Grabowski, K. M. Langner, M. Cymborowski, P. J. Porebski, P. Sroka, H. Zheng, D. R. Cooper, M. D. Zimmerman, M.-A. Elsliger, S. K. Burley and W. Minor
Acta Crystllogrphica D **72** (2016) 1181.
At the moment of publication, the database contained data from 2920 macromolecular diffraction experiments. It is intended to be expanded with more data.

Ultrafast Spin-State Dynamics in Transition-Metal Complexes Triggered by Soft-X-Ray Light
H. Wang, S. I. Bokarev, S. G. Aziz, O. Kühn,
Physical Review Letters **118** (2017) 023001.
The unprecedented short spin crossover of 4 fs, which is faster than the core-hole lifetime, has been demonstrated for L-edge excited states of a prototypical Fe(II) complex

Three-dimensional magnetization structures revealed with X-ray vector nanotomography
C. Donnelly, M. Guizar-Sicairos, V. Scagnoli, S. Gliga, M. Holler, J. Raabe, L. J. Heyderman,
Nature **547** (2017) 328.
The authors developed a hard X-ray vector nanotomography with which they imaged the 3D structure of magnetic domains of a soft magnetic pillar of diameter 5 micrometres with a spatial resolution of 100 nanometres.

Source assemblage types for cratonic diamonds from X-ray synchrotron diffraction.
F. Nestola, M. Alvaro, M. N. Casati, H. Wilhelm, A. K. leppe, A.P. Jephcoat, M. C. Domeneghetti, J. W. Harris,
Lithos **265** (2016) 334.
X-ray diffraction is used in order to determine the structure of ultrasmall inclusions in natural diamond single crystals. The non-destructive high-energy beam based approach allowed for obtaining information about chemical composition and structure of the inclusions.

Two-Photon X-Ray Diffraction
J. Stöhr,
Physical Review Letters **118** (2017) 024801.
The breakdown of conventional x-ray diffraction theory is shown for the fundamental case of a "source" consisting of a thin film back-illuminated with high incident intensity. Due to stimulated resonant scattering, the film becomes the source of cloned photon twins and the diffraction pattern becomes self-focussed beyond the diffraction limit.

Observation of the spin-polarized surface state in a noncentrosymmetric superconductor BiPd
M. Neupane, N. Alidoust, M. M. Hosen, J.-X. Zhu, K. Dimitri, S.-Y. Xu, N. Dhakal, R. Sankar, I. Belopolski, D. S. Sanchez, T.-R. Chang, H.-T. Jeng, K. Miyamoto, T. Okuda, H. Lin, A. Bansil, D. Kaczorowski, F. Chou, M. Z. Hasan, T. Durakiewicz,
Nature Comm. **7** (2016) 13315.
High-resolution angle-resolved and spin-resolved photoemission spectra probed at normal state of BiPd superconductor show the presence of Dirac point at around 700 meV below the Fermi level. The absence of spin-polarized surface states near the Fermi level negates the possibility of a topological superconducting behaviour on the surface. As such the race for topological superconductivity in noncentrosymmetric materials is ongoing.

Future conferences & workshops

ISSRNS'18
14th International School and Symposium on Synchrotron Radiation in Natural Science
Kraków (Poland), July 18-21, 2018
www.synchrotron.org.pl

Gordon Research Conference on Microscopic Probes of Intermolecular Forces and Cooperative Effects
Lucca (Italy), February 25 - March 2, 2018
www.grc.org/programs.aspx?id=15130

SRI2018
13th International Conference on Synchrotron Radiation Instrumentation
Taipei (Taiwan), June 11-15, 2018
www.nsrrc.org.tw/SRI_2018

XAFS18
17th International Conference on X-ray Absorption Fine Structure
Kraków (Poland), July 22-27, 2018
xafs2018.com

XRM 2018
14th International Conference on X-ray Microscopy
Saskatoon (Canada), August 19-24, 2018
xrm2018.com

EHPRG -56
56th European High Pressure Research Group Meeting on High Pressure Science and Technology
Aveiro (Portugal), 1-6 September 2018
www.ehprg.org/meetings.php

ESM2018
The European School of Magnetism
Kraków (Poland), 17-28 September 2018
magnetism.eu

The International Mittelwihr School on Magnetism and Synchrotron Radiation
Mittelwihr (France), October 7-12, 2018
mw2018.u-strasbg.fr

IUCR 2020
XXV Congress & General Assembly of the International Union of Crystallography
Prague (Czech Republic), August 22-30, 2020
www.iucr.org/iucr/cong/2020-iucrxxv

Find more at:
www.lightsources.org/events

Synchrotron classifieds

The webpage of PTPS (synchrotron.org.pl) was largely modified. The new structure enables easier navigation among the features. In particular we offer a space for PhD and PostDoc (http://www.synchrotron.org.pl/index.php/en/announcements/phd-studies-in-synchrotron-science) and other job position advertisements (http://www.synchrotron.org.pl/index.php/en/announcements/job-opportunities). Offers from Polish universities and research institutions are particularly welcome.

XAFS 2018

XAFS17 Conference in Kraków, Poland, 22-27.07.2018

International Conference on X-ray Absorption Fine Structure (XAFS) is organized since 1981, recently every three years. Each time it is placed in different part of the world and it was already organized by committees in USA, Japan, China and various countries in Europe. Conference is dedicated to presenting novel trends and developments in X-ray Absorption Fine Structure spectroscopy and related methods. Since XAS research is recently widely diverse, the number of presented topics is growing each time. Presentations cover both experimental applications in physics, chemistry, biology, material science, earth science and many more, but also theoretical approaches. Moreover, technical developments and new instrumentation topics are strongly represented at XAFS, with emphasis to the use of not only synchrotron sources but also x-ray free electron lasers (XFEL) and laboratory setups. Typically, presentations are divided into plenary and keynote lectures given by experts in the field as well as contributed talks and poster presentations that is also an opportunity for students and young scientists to present their work. Moreover, as satellite meetings, workshops with 'hands-on' tutorials are organized. Previous conference, XAFS16, was held in Karlsruhe, Germany, 23-28 August 2015. It gathered more than 500 scientists from various countries and it was an excellent opportunity to establish or renew collaborations and contacts with colleagues in the field.

In 2012, during XAFS15 in Beijing (China), proposals for the XAFS17 conference were briefly presented. After discussion, the IXAS Executive Committee held a closed-ballot vote to determine the conference venue. The Executive Committee voting results decided Kraków, Poland, to host XAFS17. Conference was scheduled to 22-27 July 2018.

Kraków is the second largest city in Poland and a well-established academic center with the oldest in Poland, 650-years old, Jagiellonian University and many other universities, academies, polytechnics and research institutes. In 2015 in Kraków first polish synchrotron SOLARIS (Photo 1) was commissioning and started its operation to be available for users in 2018. Kraków is also a lively city, full of cultural heritage sites (Photo 2), world-famous art and excellent cuisine.

Photo 1. Synchrotron SOLARIS building (synchrotron.pl).

Photo 2. Main Square in Kraków (wikipedia.org).

The XAFS17 is being organized by the Polish Synchrotron Radiation Society under the auspices of the International X-ray Absorption Society (IXAS) in cooperation with: Synchrotron SOLARIS, Jagiellonian University and the Henryk Niewodniczański Institute of Nuclear Physics Polish Academy of Sciences, under the honorary patronage of the Major of the City of Kraków, Rector of the Jagiellonian University and the General Director of the Institute of Nuclear Physics Polish Academy of Sciences in Kraków.

Conference venue will be placed in Auditorium Maximum of Jagiellonian University (Photo 3). Auditorium Maximum is a modern conference and teaching facility opened in 2005. It is located in close proximity to the city center. It features a six conference rooms of varying sizes and functionalities which allows to organize parallel sessions in one building. The largest room is with theatre-style seating and capacity of 1200 people (Photo 4). Auditorium Maximum is also adapted for organizing poster session.

XAFS17 program will cover all of the recent trends in x-ray spectroscopy field with lectures divided by topics, two poster sessions as well as social events – the opportunity to have discussions with colleagues, lecturers and business representatives. Conference dinner will be a chance to try excellent polish dishes and during the conference excursion you can enjoy Kraków old town, Wieliczka salt mine and many more.

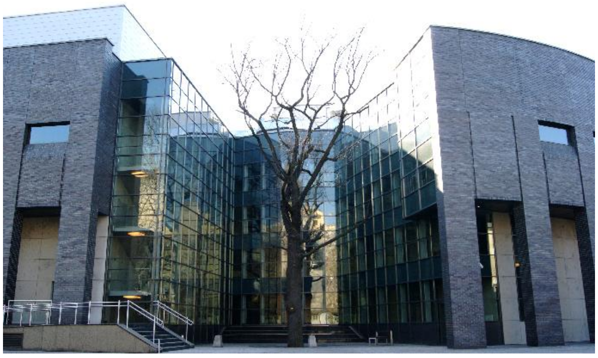

Photo 3. Auditorium Maximum building (wikipedia.org).

Photo 4. Auditorium Maximum Large Hall (konferencje.uj.edu.pl).

The Organizing Committee will be delighted to meet all scientists from all over the world who are interested in XAFS at the XAFS17 Conference in Kraków, a great place to do science and to enjoy Polish culture.

With my very best regards,

Prof. Wojciech M. Kwiatek
XAFS17 Chairman

www.xafs2018.com

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