

**International Conference**  
*"Dynamics of Systems on the Nanoscale"*



**DySoN 2023**

**Vila Lanna**  
**Prague, Czech Republic**  
**April 24-26, 2023**



**Book of Abstracts**



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## Preface

The seventh International Conference [“Dynamics of Systems on the Nanoscale”](#) (DySoN) will take place on **April 24-26, 2023**, in Vila Lanna, Prague, Czech Republic. The conference is co-organized by the [University of Kent](#) (Canterbury, United Kingdom) and [MBN Research Center](#) (Frankfurt am Main, Germany).

The DySoN Conference will be followed by the [MultiChem 2023 Conference](#) – the 2<sup>nd</sup> Annual Conference of the [COST Action CA20129 “Multiscale Irradiation and Chemistry Driven Processes and Related Technologies” \(MultiChem\)](#), which will be held on April 26-28 at the same venue.

DySoN is an interdisciplinary conference series covering a broad range of topics related to the Dynamics of Systems on the Nanoscale. The DySoN conference series was launched in 2010, and six DySoN conferences have been held [so far](#). The DySoN conferences promote the growth and exchange of interdisciplinary scientific information on the structure formation and dynamics of animate and inanimate matter on the nanometer scale. There are many examples of complex many-body systems of micro- and nanometer scale size exhibiting unique features, properties and functions. These systems may have very different nature and origins, e.g. atomic and molecular clusters, nanostructures, ensembles of nanoparticles, nanomaterials, biomolecules, biomolecular and mesoscopic systems. A detailed understanding of the structure and dynamics of these systems on the nanoscale is a difficult and fundamental task, the solution of which is necessary for nano- and biotechnologies, materials science and medicine.

Although mesoscopic, nano- and biomolecular systems differ in their nature and origin, a number of fundamental problems are common to all of them: What are the underlying principles of self-organization and self-assembly of matter at the micro- and nanoscale? Are these principles classical or quantum? How does function emerge at the nano- and mesoscale in systems of different origins? What criteria govern the stability of these systems? How do their properties change as a function of size and composition? How are their properties altered by their environment? Seeking answers to these questions is at the core of a new interdisciplinary field of Meso-Bio-Nano (MBN) Science that lies at the intersection of physics, chemistry and biology.

Experimental, theoretical, computational and applied aspects of the aforementioned problems will be discussed at the DySoN 2023 Conference. Particular attention will be devoted to dynamical phenomena and many-body effects taking place in various MBN systems on the nanoscale. They include problems of structure formation; fusion and fission; collision and fragmentation; surfaces and interfaces; collective electron excitations; reactivity; nanoscale phase and morphological transitions; irradiation-driven transformations of complex molecular systems and biodamage, channeling phenomena, and many more. Links of the DySoN topics to novel and emerging technologies will be an important focus of the conference.

Finally, DySoN 2023 will provide a platform to host discussions about current research, technological challenges and related initiatives within the Topical Areas of the DySoN conference series. The hope is that all participants will be enriched and further motivated by the session topics and the ensuing general discussions. We wish you a memorable Meeting!

### **Topical Areas of DySoN:**

- Structure and dynamics of molecules, clusters and nanoparticles
- Cluster and biomolecular ensembles, composite systems
- Clustering, self-organization, phase and morphological transitions on the nanoscale
- Nanostructured materials, surfaces and interfaces
- Reactivity and nanocatalysis
- Electron and spin transport in molecular systems
- Collision and radiation processes, fusion, fission, fragmentation
- Radiation-induced chemistry
- Irradiation-driven transformations, damage and fabrication of MesoBioNano systems
- Propagation of particles through media
- Biomedical and technological applications of radiation
- Related technologies: novel light sources, controlled nanofabrication, functionalized materials

## Conference Venue

The Conference will be hosted by Vila Lanna (V Sadech 1, 160 00 Prague 6), the conference center of the Czech Academy of Sciences located in Prague.



## Conference Reception

The conference reception will take place on Monday, April 24, from 19<sup>30</sup> to 22<sup>00</sup> and will be located at Vila Lanna.

## DySoN International Advisory Committee

- Andrey V. Solov'yov (MBN Research Center, Frankfurt am Main, Germany) - **Chair**
- Ilko Bald (University of Potsdam, Germany)
- Catherine Bréchnac (Laboratoire Aime Cotton, CNRS, Orsay, France)
- Michel Broyer (University of Lyon, France)
- Jean-Patrick Connerade (Imperial College London, London, UK)
- Franco Gianturco (The University of Innsbruck, Austria)
- Vincenzo Guidi (University of Ferrara, Italy)
- Julius Jellinek (Argonne National Laboratory, Argonne, Illinois, USA)
- Shiv Khanna (Virginia Commonwealth University, Richmond, USA)
- Nigel Mason (University of Kent, Canterbury, UK)
- Jefferson Shinpaugh (East Carolina University, Greenville, USA)
- Ilya Solov'yov (Carl von Ossietzky University, Oldenburg, Germany)
- Eugene Surdutovich (Oakland University, Rochester, Michigan, USA)

## Organizing Committee

- Andrey Solov'yov (MBN Research Center, Germany) – **Co-Chair**
- Nigel Mason (University of Kent, United Kingdom) – **Co-Chair**
- Irina Solovyeva (MBN Research Center, Germany)
- Alexey Verkhovtsev (MBN Research Center, Germany)

## Sponsors

The DySoN 2023 conference is held under the auspices of the following sponsors:

- MBN Research Center, Frankfurt am Main, Germany
- University of Kent, Canterbury, United Kingdom
- [H2020-MSCA-RISE Project “N-Light”](#)
- [H2020-MSCA-RISE Project “RADON”](#)
- [HORIZON EUROPE EIC-PATHFINDER Project “TECHNO-CLS”](#)

## Contact Information

**Prof. Dr. Andrey V. Solov'yov**  
DySoN 2023 Co-Chair

MBN Research Center gGmbH  
Altenhöferallee 3  
60438 Frankfurt am Main  
Germany  
Phone: +49 (0)69 34875600  
E-mail: [solovyov@mbnresearch.com](mailto:solovyov@mbnresearch.com)  
Website: [www.mbnresearch.com](http://www.mbnresearch.com)

**Professor Nigel J. Mason, OBE**  
DySoN 2023 Co-Chair

School of Physics and Astronomy  
University of Kent  
Canterbury, CT2 7NH  
United Kingdom  
Phone: +44 (0)1227 823321  
E-mail: [N.J.Mason@kent.ac.uk](mailto:N.J.Mason@kent.ac.uk)  
Website: <https://www.kent.ac.uk/physics-astronomy>

## DySoN Conference Web Page

Updated information on the DySoN 2023 conference is available at [www.dyson-conference.org](http://www.dyson-conference.org). General information on the DySoN conference series can also be found there.



## Conference Program

*Monday, April 24*

08 <sup>00</sup> – 09 <sup>00</sup>	Participants registration
09 <sup>00</sup> – 09 <sup>10</sup>	<b>DySoN 2023 Opening</b>
09 <sup>10</sup> – 11 <sup>00</sup>	<p><b><u>Morning session I: Dynamics of systems on the nanoscale (Chair: Nigel J. Mason)</u></b></p> <p><b>Andrey Solov'yov</b>, MBN Research Center, Frankfurt am Main, Germany <i>Reactive and irradiation driven molecular dynamics research breakthroughs with MBN Explorer</i></p> <p><b>Ilko Bald</b>, Institute of Chemistry, University of Potsdam, Germany <i>Hybrid nanostructures for sensitive surface-enhanced Raman scattering (SERS) and plasmonic chemistry</i></p> <p><b>Eric Suraud</b>, Laboratoire de Physique Théorique, Université de Toulouse, France <i>(Un)expected behaviors of small molecules after (ultra)fast XUV irradiation</i></p> <p><b>Hidetsugu Tsuchida</b>, Quantum Science and Engineering Center, Kyoto University, Japan <i>Radiolysis of liquid water occurring around ion tracks of carbon beams</i></p>
11 <sup>00</sup> – 11 <sup>20</sup>	Coffee break
11 <sup>20</sup> – 13 <sup>10</sup>	<p><b><u>Morning session II: Structure and dynamics of biomolecular and biological systems (Chair: Ilia A. Solov'yov)</u></b></p> <p><b>Michael Hausmann</b>, Kirchhoff-Institute for Physics, Heidelberg University, Germany <i>Functionally determined spatial organisation of receptors and proteins integrated in bi-lipid membranes of cells</i></p> <p><b>Martin Falk</b>, Institute of Biophysics, Czech Academy of Sciences, Brno, Czech Republic <i>Update on the relationship between the architecture of repair foci (IRIF) and DSB repair</i></p> <p><b>Marc Benjamin Hahn</b>, Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany <i>The change of DNA and protein radiation damage upon hydration: In-situ observations by near-ambient-pressure XPS</i></p> <p><b>Dorothea Hallier</b>, Fraunhofer Institute for Cell Therapy and Immunology, Potsdam, Germany <i>X-ray damage to Gene-V Protein: UHV and NAP-XPS analysis of Chemical changes to Proteins</i></p>
13 <sup>10</sup> – 14 <sup>30</sup>	Lunch
14 <sup>30</sup> – 16 <sup>10</sup>	<p><b><u>Afternoon session I: Structure and dynamics of molecules, clusters and nanoparticles (Chair: Ilko Bald)</u></b></p> <p><b>Luca Gerhards</b>, Carl von Ossietzky University Oldenburg, Germany <i>Spin dynamics and spin relaxation in biological systems – Introducing MolSpin as versatile toolkit</i></p> <p><b>Robin Schürmann</b>, Physikalisch-Technische Bundesanstalt, Berlin, Germany <i>Elucidating chemical reactions on nanoparticles by synchrotron X-ray-techniques</i></p> <p><b>Anushree Dutta</b>, Institute of Chemistry, University of Potsdam, Germany <i>Kinetics and mechanism of plasmon driven dehalogenation reaction of brominated nucleobases</i></p>

	<b>Vasyl Shvalya</b> , Jožef Stefan Institute, Ljubljana, Slovenia <i>Bacterial DNA distinctive SERSing with plasma-printed nanogold</i>
16 <sup>10</sup> – 16 <sup>30</sup>	Coffee break
16 <sup>30</sup> – 18 <sup>30</sup>	<b><u>Afternoon session II: Clustering, self-organization, phase and morphological transitions on the nanoscale (Chair: Beata Ziaja-Motyka)</u></b>  <b>Wolfgang Ernst</b> , Graz University of Technology, Austria <i>Mixed-metal nanoparticles – core-shell structures, phase transitions and alloying</i>  <b>Felipe Fantuzzi</b> , University of Kent, Canterbury, United Kingdom <i>Unraveling structural changes in graphene and lithium fluoride nanostructures: Insights from reactive and Born-Oppenheimer molecular dynamics simulations</i>  <b>Miloš Baljžović</b> , Swansea University, United Kingdom <i>Imaging neuromorphic dynamics of percolating nanocluster networks</i>  <b>Theodoros Pavloudis</b> , Swansea University, United Kingdom <i>Multiscale modeling of Au-C nanostructured systems: Nanoparticle shapes and neuromorphic dynamics</i>
19 <sup>30</sup> – 22 <sup>00</sup>	Welcome reception

## ***Tuesday, April 25***

09 <sup>00</sup> – 10 <sup>50</sup>	<b><u>Morning session I: Nanostructured materials, surfaces and interfaces (Chair: Wolfgang Ernst)</u></b>  <b>Andrew Wheatley</b> , University of Cambridge, United Kingdom <i>Dual control of morphology and composition in heterobimetallic catalysts for oxygen reduction</i>  <b>David Field</b> , Aarhus University, Denmark <i>The challenge of the spontelectric state</i>  <b>Vincenzo Guidi</b> , University of Ferrara, Italy <i>Reversible chemisorption of gases on nanostructures for gas sensing</i>  <b>Agata Kowalska</b> , Maritime University in Szczecin, Poland <i>XRD and PAS investigation of crystal lattice defects induced in Zr by low energy deuterons</i>
10 <sup>50</sup> – 11 <sup>20</sup>	Coffee break
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13 <sup>10</sup> – 14 <sup>30</sup>	Lunch



14 <sup>30</sup> – 16 <sup>00</sup>	<p><b>Afternoon session I: Reactivity and nanocatalysis (Chair: Andrew Wheatley)</b></p> <p><b>Dmitry Momotenko</b>, Carl von Ossietzky University Oldenburg, Germany <i>Electrochemical nanotechnology: 3D printing of metals at the nanoscale</i></p> <p><b>Rodolphe Antoine</b>, Université Claude Bernard Lyon1, France <i>Reactive oxygen species produced upon photoexcitation of monolayer protected noble metal clusters. From in silico to in vitro</i></p> <p><b>Shiv Khanna</b>, Virginia Commonwealth University, USA <i>Stable metal-chalcogenide clusters for nano p- n- junction with tunable band gaps, adjustable band alignment, light harvesting and CO<sub>2</sub> activation</i></p>
16 <sup>00</sup> – 16 <sup>30</sup>	Coffee break
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	<p><b>Laura Bandiera</b>, Istituto Nazionale di Fisica Nucleare, Ferrara, Italy  <i>Channeling radiation experiments with multi-GeV electron and positron beams: recent results and future perspectives</i></p>
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## Reactive and irradiation driven molecular dynamics research breakthroughs with MBN Explorer

Andrey V. Solov'yov

MBN Research Center, Altenhöferallee 3, 60438 Frankfurt am Main, Germany  
E-mail: solovyov@mbnresearch.com

The standard classical molecular dynamics approach does not describe explicitly the electron dynamics and, therefore, most of the quantum transformations that may occur during the system motion. These transformations are often induced in the system through exposure to external perturbations such as external fields, or irradiation by charged particles (electrons, protons, ions, etc) or photons, or due to chemical reactions. The resulting effects may have a global character (electric current, spin ordering, polarisation, magnetisation, etc) or be local (atomic or molecular excitation, ionisation, dissociation, charge transfer, etc).

Reactive or irradiation induced local quantum perturbations of a molecular system typically occur on the sub-femtosecond to the femtosecond time scale and often involve only those atoms that are directly affected by the irradiation or chemical processes. Such processes typically involve the nearest environment of the targeted molecular sites, being a small part of the entire molecular system, and happen within femtoseconds or even faster. The femtosecond time scale is, however, significantly shorter than characteristic timescales of motion of multi-atomic molecular systems, as the typical integration time step in classical molecular dynamics simulations of such systems is ~1-2 fs.

Coupling of local, rapid quantum transformations that may occur within classically moving large molecular systems has been accomplished in reactive molecular dynamics (RMD) and irradiation driven molecular dynamics (IDMD) [1,2]. In both cases the classical MD is superimposed with random quantum transformations that may occur in a molecular system in the course of its classical motion. Examples of transformations include breakages of interatomic bonds occurring either due to the system irradiation or chemical reactions, charge transfers, change of atomic properties, such as interatomic interaction potentials, valences of atoms, formation of excited atoms, ions, etc. Such possibilities can be introduced into the MD framework by means of reactive CHARMM force field (rCHARMM) [2]. The rCHARMM force field, RMD and IDMD have been implemented in the advanced software package MBN Explorer [3].

The talk will introduce the principles of RMD, IDMD and rCHARMM force field as well as their implementation in the MBN Explorer which is supplemented with the powerful multitask toolkit MBN Studio [4]. It will give an overview of the recent case studies and related research breakthroughs achieved with the aforementioned techniques and computational tools, which include atomistic simulations of focused electron induced deposition processes (see [5] and references therein) and ion beam induced DNA damage processes within cells (see [6] and references therein). Particular emphasis will be made on the elucidation of multiscale nature of the discussed irradiation driven and chemical processes, their quantitative description, as well as on verification of the results of simulations through various experiments. A brief survey of areas of application of the aforementioned techniques will be presented following the recent publications [7,8].

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## Hybrid nanostructures for sensitive surface-enhanced Raman scattering (SERS) and plasmonic chemistry

Ilko Bald, Kosti Tapio, Sergio Kogikoski Jr., Anushree Dutta, Amr Mostafa, Yuya Kanehira

Institute of Chemistry, University of Potsdam,  
Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany  
E-mail: bald@uni-potsdam.de

DNA origami nanostructures are ideally suited to arrange both plasmonic nanoparticles as well as receptors for analyte molecules with nanometer precision. Thus, they can be exploited for surface-enhanced Raman scattering (SERS), where the strongest signal enhancement is localized in nanometric hot spots and where the DNA origami can be used to precisely position the molecules of interest. In recent years we have demonstrated the few- and single-molecule SERS detection in different nanoparticle arrangements [1-4]. We have created a dedicated DNA origami nanoantenna [4], which was also used to study chemical changes in hemin [5], and to detect single proteins [4].

In the present contribution we demonstrate the further optimization of the nanoantenna by comparing the SERS performance of dimers of different nanoparticle species from spherical Au and Ag nanoparticles to anisotropic gold nanoflowers and combinations thereof. A combination of Au nanoflower and Ag nanosphere allows for a broadband SERS excitation and improved single-molecule detection.

With these structures at hand we studied systematically how SERS spectra are modified when transitioning from bulk spectra over few molecules up to the single molecule level. Latest measurements from small molecules as well as proteins will be shown.

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**(Un)expected behaviors of small molecules after (ultra)fast XUV irradiation**

P.-G. Reinhard<sup>1</sup>, D. Dundas<sup>2</sup>, P. M. Dinh<sup>1</sup>, M. Vincendon<sup>1</sup>, E. Surraud<sup>1,2</sup>

<sup>1</sup>Institut fuer Theoretische Physik, Universitaet Erlangen, Staudtstrasse 7, Erlangen, Germany

<sup>2</sup>School of Mathematics and Physics, Queen's University Belfast, UK

<sup>3</sup>Laboratoire de Physique Théorique, Université de Toulouse, CNRS, UPS, France

Email: [surraud@irsamc.ups-tlse.fr](mailto:surraud@irsamc.ups-tlse.fr)

We review several investigations of ultrafast irradiation of small molecules in dedicated pump and probe setups. We first consider the usual long IR pump followed by an XUV attosecond train and analyze the physical content of the ionization signals. We consider both global signals such as the total ionization and angular and/or energy resolved ionization. All signals deliver similar regular pattern mostly reflecting the characteristics of the IR pump. We next release the technical constraints of the attosecond train and consider a short IR pump followed by a single attosecond XUV probe (no train) to avoid bias toward the properties of the IR pump. We again analyze the ionization characteristics and try to link them to specific properties of the target system.

We finally investigate the depletion of single-electron states in small molecules under the influence of very short XUV pulses. For some XUV energies we observe a marked occupation inversion, where depletion of the deep bound state becomes much larger than other ones. This drives a dipole instability, i.e. a spontaneous reappearance of the dipole signal long after the laser pulse is over and the dipole signal has died out. The dipole signal that emerges from this instability can be identified as a particular low-energy structure in photo-electron spectra. This instability can be explored simplifying the excitation mechanism by instantaneous generation of a hole in one of the occupied states of the system. We investigate how the dipole instability depends on the system, the state in which the hole is cut, and the amount of depletion which is given to the hole state. The mechanism might appear in other systems described by mean field approaches although the role of dynamical correlations might not be the definitive key here.

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## Radiolysis of liquid water occurring around ion tracks of carbon beams

Hidetsugu Tsuchida<sup>1,2,\*</sup>, Tomoya Tezuka<sup>2</sup>, Takeshi Kai<sup>3</sup>, Yusuke Matsuya<sup>3,4</sup>, Takuya Majima<sup>2</sup>,  
Manabu Saito<sup>1,2</sup>

<sup>1</sup>Quantum Science and Engineering Center, Kyoto University, Gokasho, Uji, Kyoto, 611-0011, Japan

<sup>2</sup>Department of Nuclear Engineering, Kyoto University, Nishikyo-ku, Kyoto, 614-8530, Japan

<sup>3</sup>Nuclear Science and Engineering Center, Japan Atomic Energy Agency, 2-4 Shirakata Shirane, Tokai-mura, Naka-gun, Ibaraki, 319-1195, Japan

<sup>4</sup>Faculty of Health Sciences, Hokkaido University, Kira-12 Nishi-5, Kita-ku, Sapporo, Hokkaido, 060-0812, Japan

\*E-mail: tsuchida@nucleng.kyoto-u.ac.jp

The biological effects after radiation exposure are known to be caused by the action of water radiolysis products on DNA. Among various radiation types, fast ion beams cause high ionizing events and damage living organisms. This effect (such as cell killing and mutation) induced by DNA damage has been used for radiotherapy and plant breeding. Since liquid water is the main component of biological matter, many recent studies have focused on clarifying the role of liquid water in the DNA damage process by the fast ion beam [1,2]. For this end, it is essential to understand the elementary process of water radiolysis around the ion tracks.

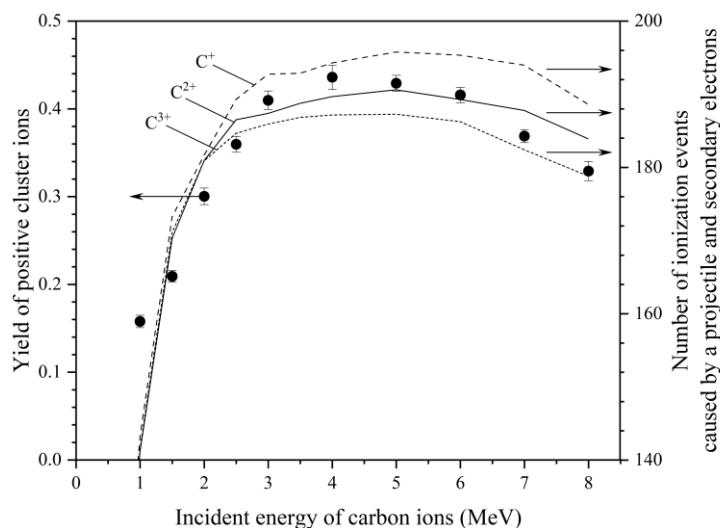
Here, we report the experimental and simulation results on ion-induced water radiolysis. We measured secondary ions produced during irradiating liquid water with fast ion beams. In this experiment, a target of pure water was introduced into a vacuum by the liquid molecular beam method and was irradiated with a carbon ion beam of 1.0 to 8.0 MeV (1–3 MeV C<sup>+</sup>, 4–6 MeV C<sup>2+</sup>, and 7–8 MeV C<sup>3+</sup>), corresponding to that appearing at Bragg peak region. The secondary ions from the target were measured with a time-of-flight mass spectrometer. We studied the dependence of the secondary ion yield on the incident energy of the carbon ions.

The main positive charge products were the water cluster ions (H<sub>2</sub>O)<sub>n</sub>H<sub>3</sub>O<sup>+</sup> ( $n = 0-5$ ) with H<sub>3</sub>O<sup>+</sup> as the nucleus. These ions are produced by ion-molecule reactions between ionized H<sub>2</sub>O<sup>+</sup> ions and surrounding water molecules. Based on this result, the ionization of liquid water by carbon ion irradiation was analyzed using the track-structure simulation code PHITS (Particle and Heavy Ions Transport code System). In this simulation, we investigated how incident ions and secondary electrons are involved in water ionization events in liquid water in the region of secondary ion escape depth. Figure 1 plots the positive water cluster ion yield as a function of incident carbon ion energy. The yield increases with increasing incident energy, reaches a maximum around 4 MeV, and then decreases gradually. We found that this dependence follows the same trend as that calculated by PHITS shown in Fig. 1, which is the number of ionization events generated by incident ions and secondary electrons. The analysis also showed that about 70% of the ionization was due to secondary electrons, with secondary electron energies ranging from 10.9 to 600 eV.

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**Figure 1:** Comparison of the relationship between the incident carbon energy and the positive water cluster ion yield (left of the vertical axis, filled circle symbols) and the number of ionizations generated by incident ions and secondary electrons calculated by PHITS (right of the vertical axis, lines). Different lines represent different charge states of incident carbon.

**Functionally determined spatial organisation of receptors and proteins  
integrated in bi-lipid membranes of cells**

Michael Hausmann

Kirchhoff-Institute for Physics, Heidelberg University,  
Im Neuenheimer Feld 227, 69120 Heidelberg, Germany  
E-mail: hausmann@kip.uni-heidelberg.de

The formation of lipid membranes in water environment is physically determined by entropy and thermodynamic forces. Cell membranes separate an inner cell reaction volume from outside, but allow cell-cell communication, ion transports and opening and closing of channels by integrated receptor and protein molecules. For the optimal integration of these molecules into the lipid arrangement of the membrane, an adaptation of the membrane thickness to the hydrophobic parts of the molecules is required. Computer simulations have shown that this reasons that the molecular axis of receptors stands approximately perpendicular to the membrane plane. Moreover, due to thermodynamic energy conditions receptors and proteins integrated into membranes arrange in similarly sized clusters. These clusters change in size when ligands bind to receptors or medical treatments are applied to cells. By means of super-resolution fluorescence localization microscopy cluster formation and treatment dependent cluster (re-)arrangements are investigated for ErbB-receptors in breast cancer and glioblastoma cell lines. The data reveal how these changes in clustering correlate with receptor-pairing and internalization into the cells. By this way heregulin binding to Erb-B2 indirectly stimulates changes in chromatin organization which are correlated to gene activation. In addition, different medical treatments and their impact on membrane molecule organization were studied. As an example, it is shown how the application of local anesthetics impacts the organization of ryanodine receptors. Other examples show how peritoneal dialysis fluids influence the spatial organisation and clustering of the tight junction proteins zonula occludens-1 and claudin-5 accompanied by changes in transport rates were quantified in the endothelial cell membrane. In conclusion, the results of the presented investigations show that molecular self-organisation driven by physical laws of thermodynamics has functional importance in cell membranes and cells.

**Update on the relationship between the architecture of repair foci (IRIF)  
and DSB repair**

Martin Falk<sup>1,2</sup>, Jiří Toufar<sup>1</sup>, Michael Hausmann<sup>2</sup>, Charlotte Nietzel<sup>2</sup>, Olga Kopečná<sup>1</sup>, Tomáš Vičar<sup>3</sup>, Hannes Hahn<sup>2</sup>, Lucie Dobešová<sup>1</sup>, Iva Falková<sup>1</sup>, Götz Pilarczyk<sup>2</sup>, Theresa Gier<sup>2</sup>, Alena Bačková<sup>1</sup>

<sup>1</sup>Institute of Biophysics, The Czech Academy of Sciences, Brno, Czech Republic

<sup>2</sup>Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany

<sup>3</sup>Department of Biomedical Engineering, Faculty of Electrical Engineering and Communication, Brno University of Technology, Czech Republic

E-mail: falk@ibp.cz

The accumulating results suggest that the architecture of biomolecular complexes and networks plays a significantly more important role in regulating and mediating cellular processes than previously thought. An illustrative example is the regulation and efficiency of DNA repair after radiation damage. Our results suggest that chromatin architecture influences the formation of repair complexes (ionizing radiation-induced foci, IRIF) at DNA double-strand breaks (DSBs), which subsequently co-determine the efficiency of repair processes by their architecture, and presumably participate in the selection of repair mechanisms at the sites of individual DSBs. In this talk, we will present new tools for describing the micro- and nano-architecture of chromatin and IRIF, as well as results concerning the link between chromatin architecture, architecture of gH2AX foci and selected repair proteins (53BP1, RAD51), and repair processes in normal and radioresistant cancer cells.

Acknowledgements: COST MultiChem Project, Action CA20129

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**The change of DNA and protein radiation damage upon hydration:  
In-situ observations by near-ambient-pressure XPS**

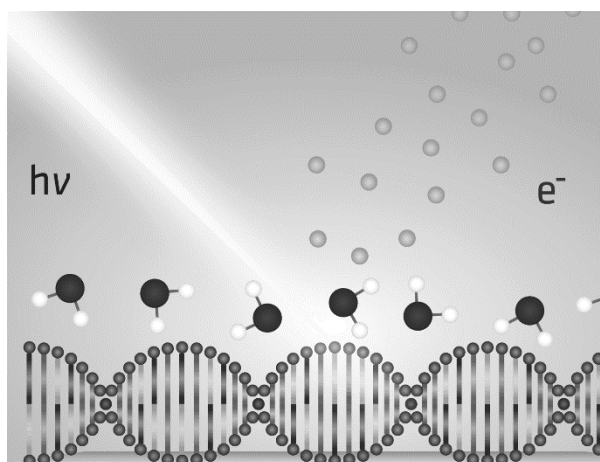
Marc Benjamin Hahn<sup>1</sup>, Dorothea C. Hallier, Paul M. Dietrich<sup>2</sup>, Jörg Radnik<sup>1</sup>

<sup>1</sup>Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany.

<sup>2</sup>SPECS Surface Nano Analysis GmbH, Berlin, Germany

E-mail: marc-benjamin.hahn@fu-berlin.de

X-ray photoelectron-spectroscopy (XPS) allows simultaneous irradiation and damage monitoring. Although water radiolysis is essential for radiation damage, all previous XPS studies were performed in vacuum. [1] Here we present near-ambient-pressure XPS experiments to directly measure DNA damage under water atmosphere. They permit in-situ monitoring of the effects of radicals on fully hydrated double-stranded DNA. Our results allow us to distinguish direct damage, by photons and secondary low-energy electrons (LEE), from damage by hydroxyl radicals or hydration induced modifications of damage pathways. The exposure of dry DNA to x-rays leads to strand-breaks at the sugar-phosphate backbone, while deoxyribose and nucleobases are less affected. In contrast, a strong increase of DNA damage is observed in water, where OH-radicals are produced. In consequence, base damage and base release become predominant, even though the number of strand-breaks increases further.



**Figure 1:** X-rays interact with hydrated DNA and eject photoelectrons. With permission from Ref. [1].

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**X-ray damage to Gene-V Protein:  
UHV and NAP-XPS analysis of Chemical changes to Proteins**

Dorothea C. Hallier<sup>\*,1,2,3</sup>, Jörg Radnik<sup>2</sup>, Paul M. Dietrich<sup>4</sup>, Harald Seitz<sup>1,3</sup>, Marc Benjamin Hahn<sup>2</sup>

<sup>1</sup>Fraunhofer Institute for Cell Therapy and Immunology, Branch Bioanalytics and Bioprocesses,  
Am Mühlenberg 13, 14476 Potsdam, Germany

<sup>2</sup>Federal Institute for Materials Research and Testing BAM,  
Unter den Eichen 87, 12205 Berlin, Germany

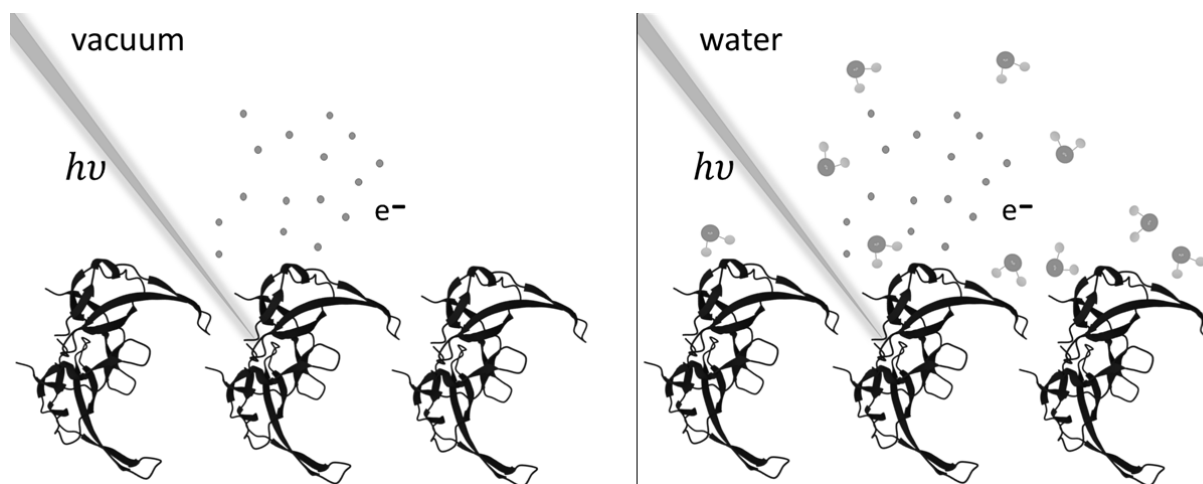
<sup>3</sup>University of Potsdam, Institute for Biochemistry and Biology,  
Karl-Liebknecht-Straße 24-25, 14476 Potsdam, Germany

<sup>4</sup>SPECS Surface Nano Analysis GmbH,  
Voltastraße 5, 13355 Berlin, Germany

\*E-mail: dorothea.hallier@izi-bb-extern.fraunhofer.de

X-ray photoelectron spectroscopy (XPS) was used to analyze the chemical damage of ionizing radiation to a single-stranded DNA-binding protein: Gene-V Protein (G5P/GVP) and its most abundant amino acids (Alanine, Arginine, Cysteine, Glycine, Lysine, Methionine, Tyrosine). This protein plays a crucial role in maintaining Bacteriophage F1, especially its DNA replication, recombination and repair. Hence, G5P serves as a model protein for ssDNA-binding proteins.

Vacuum (UHV) measurements were combined with near-ambient pressure (NAP) XPS measurements under water and nitrogen atmosphere to detect both direct and indirect radiation damage to G5P protein and selected aminoacids as well as corresponding damage pathways. The exposure of proteins and aminoacids to x-rays led to degradation i.e. via dehydrogenation, decarboxylation, dehydration and deamination. Furthermore, reactive neutral or ionic radicals derived upon protein fragmentation. A strong increase of protein damage was observed in water as compared to vacuum.



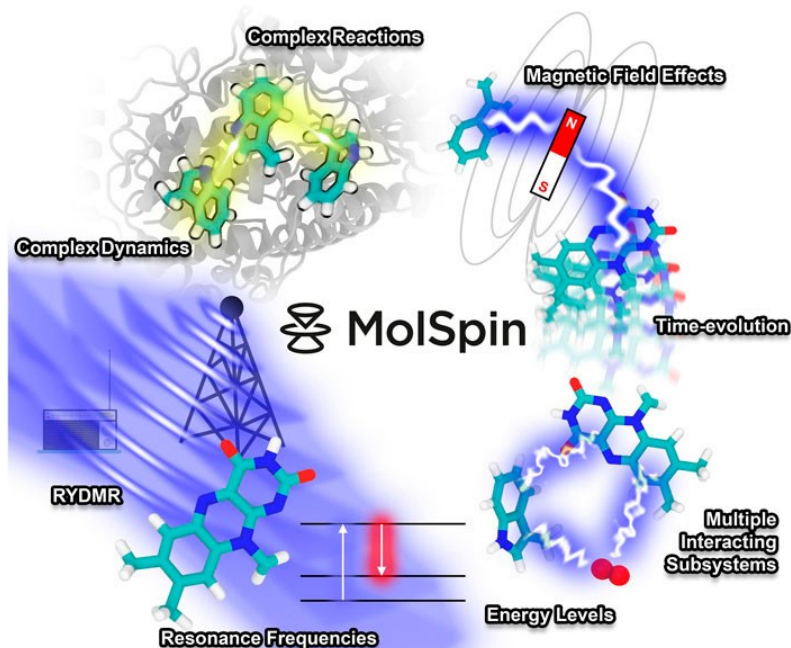
**Figure 1:** X-rays pass through vacuum (left) or water atmosphere (right), scatter at the Gene-V Protein (G5P) and eject photoelectrons.

## Spin dynamics and spin relaxation in biological systems – Introducing MolSpin as versatile toolkit

Luca Gerhards, Ilia A. Solov'yov

Institute of Physics, Carl-Von-Ossietzky University  
Carl-Von-Ossietzky Straße 9-11, 26129, Oldenburg, Germany  
E-mail: luca.gerhards@uni-oldenburg.de  
E-mail: ilia.solovyov@uni-oldenburg.de

Spin-dependent chemical reactions reveal fascinating mechanisms which are of high interest in the current scientific community. For instance, the application of an external magnetic field would affect the yield in simple radical reactions of formic acid formation [1]. Furthermore, spin-dependent reactions are believed to be the fundamental cause for several biological processes such as magnetoreception in migratory species or crucial processes in photosynthesis [2, 3]. It is thus important to understand and describe the dynamics and interactions of spin systems of varied complexity. Not only the interactions between spins but also the influence of the environment exhibits an important aspect which leads to observable effects in experiments. The underlying theoretical framework to describe these effects relies on the Liouville-Von Neumann equation. However, the solution of this equation is in most cases not only challenging for realistic systems but also requires the utilization of supercomputers.



**Figure 1:** Examples of problems that can be described by MolSpin [4].

We have developed the software package MolSpin to efficiently solve and investigate spin dynamics for spin chemistry problems [4]. With MolSpin it is possible to describe spin-dependent reaction mechanisms, the influence of molecular motion and other perturbations using the Bloch-Redfield-Wangsness formalism, and several other features. The software package is built to allow for an easy implementation of additional tasks and is thus suitable for challenging problems related to spin dynamics.

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## Elucidating chemical reactions on nanoparticles by synchrotron X-ray-techniques

Robin Schürmann<sup>1</sup>, Aleksandar Milosavljevic<sup>2</sup>, Ilko Bald<sup>3</sup>, Christian Gollwitzer<sup>1</sup>

<sup>1</sup>7.2 "X-ray Metrology with Synchrotron Radiation", Physikalisch-Technische Bundesanstalt (PTB),

Abbestr. 2-12, 10587, Berlin, Germany

<sup>2</sup>PLEIADES beamline, Synchrotron SOLEIL,

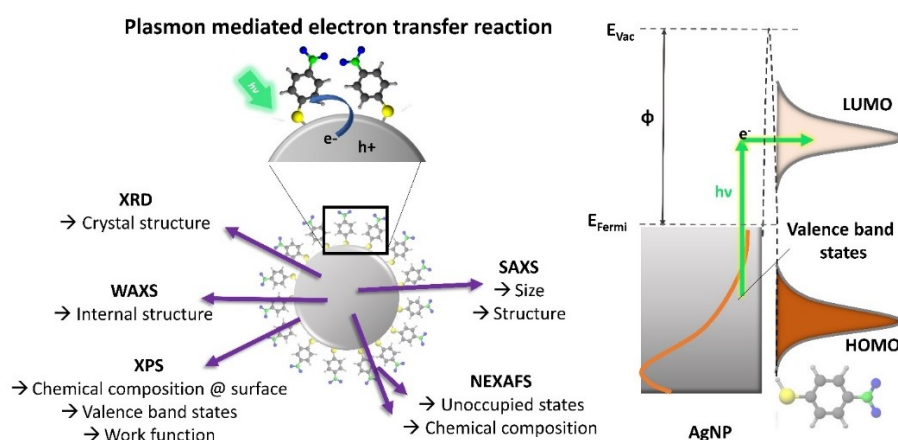
L'Orme des Merisiers, 91190, Saint-Aubin, France

<sup>3</sup>Institute of Chemistry, University Potsdam,

Karl-Liebknecht-Str. 24-25, 14476, Potsdam, Germany

E-mail: robin.schuermann@ptb.de

Nanoparticles (NPs) provide versatile applications to drive chemical reactions on their surface that are induced by light, heat or electrons. Collective oscillations of the conduction-band electrons in noble-metal NPs can be excited by visible light and generate electron-hole pairs in a non-radiative decay pathway. Such low energy electrons can be transferred to adsorbed ligand molecules on the NP surface and trigger reactions therein. The electron transfer probability depends on the initial and final electronic states and the work function of the NP-ligand-system. However, the electronic properties at the metal-organic-interface are highly influenced by the NP-ligand interaction and may differ significantly from their bulk properties [1]. To obtain a comprehensive picture of the properties determining the reaction kinetics and products, a detailed knowledge of the material properties is required. Complementary synchrotron-based X-ray absorption and scattering techniques allow the measurement of relevant properties of the NP-ligand system. X-ray photoelectron spectroscopy (XPS) of isolated AuNPs provided a detailed understanding on the role of electronic states in plasmon mediated reactions [2,3].



**Figure 1:** Properties of NP-ligand systems that can be measured by (synchrotron-based) X-ray techniques (left) and the electronic properties defining the electron transfer probability in illuminated ligand coated AgNPs (right)

Beside the electronic properties also the morphology and internal structure of the nanoparticles need to be measured with high accuracy, since in catalytical applications NPs with increasing complexity are used. In a recent study, poly(ionic liquid) nanovesicles (NVs) with multilamellar structure and decorated with CuNPs have been used for CO<sub>2</sub> electroreduction.[4] In such systems the shell thickness is essential in regulating the shape robustness and mass transport into and out of NVs. Therefore, small- and wide-angle X-ray scattering (SAXS/WAXS) have been used to measure the dimensional properties of the NVs, which are determining the reaction products and yield.

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## Kinetics and mechanism of plasmon driven dehalogenation reaction of brominated nucleobases

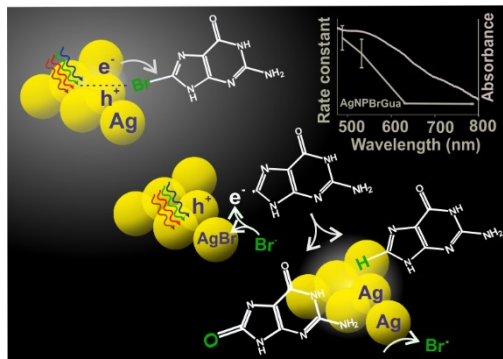
Anushree Dutta<sup>1</sup>, Robin Schürmann<sup>1</sup>, Sergio Kogikoski Jr.<sup>1</sup>,  
Niclas. S. Mueller<sup>2</sup>, Stephanie Reich<sup>2</sup>, Ilko Bald<sup>1</sup>

<sup>1</sup>Institute of Chemistry, University of Potsdam,  
Karl-Liebknecht-Str. 24-25, 14476, Potsdam, Germany.

<sup>2</sup>Department of Physics, Freie Universität Berlin,  
Arnimallee 14, 14195 Berlin, Germany

E-mail: anushree.dutta@uni-potsdam.de; ilko.bald@uni-potsdam.de

A dehalogenation kinetics of 8-bromoguanine (BrGua) and 8-bromoadenine (BrAde) on the aggregated surfaces of silver (Ag) and gold (Au) NPs have been studied and monitored by surface enhanced Raman scattering (SERS). [1] Based on a proposed kinetic model, we infer that the time-average constant concentration of hot electrons and the time scale of dissociation of transient negative ions (TNI) are crucial in defining the reaction rate law. Based on this, a pseudo first order reaction rate law is proposed. [1],[2] An overall higher reaction rate of dehalogenation is observed on Ag compared with Au, which is explained by the favorable hot-hole scavenging by the reaction product and the byproduct. It is concluded that the insufficient hole deactivation could retard the reaction rate significantly, marking itself as rate-determining step for the overall reaction. The nonthermal nature of the plasmon driven reaction is understood from the wavelength dependency of the reaction rate normalized to absorbed optical power. Further we observe that the dehalogenation reaction rate law is independent of the nature of brominated purines and the Au and Ag substrate. The feasibility of the reaction and their corresponding reaction rate is guided by nature of the brominated purines and the plasmonic substrate involved.



**Figure 1:** Schematic depiction of aggregated Ag surface for Plasmon driven dehalogenation reaction of brominated purines.

The study not only provides a better understanding of the reactivity of brominated purine derivatives on the aggregates of Ag and Au, but also lays a general understanding of the kinetics and reaction mechanism of a plasmon-driven reaction in a heterogeneous system.

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## Bacterial DNA distinctive SERSing with plasma-printed nanogold

V. Shvalya<sup>1</sup>, M. Modic<sup>1</sup>, M. Abutoama<sup>2</sup>, J. Zavašnik<sup>1</sup>, C. Skubic<sup>3</sup>,  
N. Nadižar<sup>3</sup>, D. Rozman<sup>3</sup>, U. Cvelbar<sup>1</sup>

<sup>1</sup>Department of Gaseous Electronics (F6), Jožef Stefan Institute, Jamova cesta 39,  
SI-1000 Ljubljana, Slovenia

<sup>2</sup>Department of Electrooptics and Photonics Engineering and the Ilse Katz Center for Nanoscale Science and  
Technology, School of Electrical and Computer Engineering, Ben-Gurion University of the Negev, Beer  
Sheva 84105, Israel

<sup>3</sup>Centre for Functional Genomics and Bio-Chips, Institute of Biochemistry and Molecular Genetics, Faculty  
of Medicine, University of Ljubljana, Zeloška 4. SI-1000 Ljubljana, Slovenia  
E-mail: VasyI.Shvalya@ijs.si

Optical sensing substrates for structural analysis of biological supermolecules such as RNA or DNA are of great scientific interest in nanomedicine and nanobiotechnology [1]. Surface-enhanced Raman scattering (SERS) is the optical technique that enables nondestructive, rapid, and label-free diagnosis of DNA monolayers and relevant biomembranes in nanovolumes. To be efficient, SERS requires a significant improvement in photon scattering processes, which can be achieved by using advanced nanoplasmonic accessories. These substrates, which are preferably noble metals, and in the case of biomaterials study it is gold, significantly increase the molecular scattering cross-section due to the field confinement effect and the interaction with the analyte on the metal surface [2]. Here, plasma was used as a tool to design a nanoplasmonic optical sensor by following an accelerated electrochemical reduction mechanism according to which nanogold aggregates were obtained from an evaporated aqueous solution containing an ionic metal precursor. The generated nanostructures showed an advanced analytical response (the amplification factor is of the order of  $10^7$ ), and the sensitivity of the chip allowed us to obtain Raman fingerprints of isolated bacterial DNA fragments within a few seconds. The collected spectral data from *Escherichia coli*, *Janthinobacterium lividum*, *Micrococcus luteus*, and *Staphylococcus aureus* allowed us to estimate the genomic content of nucleobases in the DNA molecule at a nanogram sample size. The results were compared with long-term whole-genome sequencing of the bacterial strains using Oxford Nanopore technology. Finally, based on the major DNA molecular fingerprint features reflected by the different peak intensities of adenine (A), guanine (G), cytosine (C), and thymine (T), statistical principal component analysis was successfully used to quickly, effortlessly, and reliably distinguish the bacterial strains [3].

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## Mixed-metal nanoparticles – core-shell structures, phase transitions and alloying

Wolfgang E. Ernst, Andreas W. Hauser

Institute of Experimental Physics, Graz University of Technology,  
Petersgasse 16, 8010 Graz, Austria  
E-mail: wolfgang.ernst@tugraz.at

Nanoparticles of a few nanometer diameter consisting of different materials in layered core@shell structures are synthesized by sequential doping of cold helium droplets in a molecular beam apparatus and deposited on solid carbon, h-BN, or SiN substrates [1]. After surface deposition, the samples are removed and various measurement techniques are applied to characterize the created particles: scanning transmission electron microscopy at atomic resolution, electron tomography, temperature dependent STEM and TEM up to 1000 degree C, energy-dispersive x-ray spectroscopy (EDXS), electron energy loss spectroscopy (EELS), optical absorption, and photoelectron spectroscopy[1,2]. Our investigations have included alloy formation at high temperature as well as the chemical reactivity and stability of Ni, Fe, and Co cores of 2 to 3 nm diameter passivated by a few layers of gold [3]. Combinations of a plasmonic core and a metal oxide shell exhibit enhanced photoelectron yields with impact on the catalytic properties of the nanoparticles [2]. A plasmonic core also influences the fluorescence properties of a shell material. Fluorescence quenching or enhancement in Rhodamine B covered Au nanoparticles was observed depending on the thickness of an intermediate molecular layer of a dielectric material between the Au core and the RhB shell [4].

On the way towards cluster catalytic experiments, we have shown that  $V_2O_5$  nanoparticles can be generated by sublimation from the bulk [5] and deposited while keeping the original stoichiometry [6]. Our attempts to create Au- $V_2O_5$  core-shell particles in the way described above, did not yield the expected encapsulated structure but after deposition, Janus particles of Au and  $V_2O_5$  with radii of about 20 nm were identified [7].

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## Unraveling structural changes in graphene and lithium fluoride nanostructures: Insights from reactive and Born-Oppenheimer molecular dynamics simulations

Felipe Fantuzzi

School of Chemistry and Forensic Science, University of Kent,  
Park Wood Rd, Canterbury CT2 7NH, UK  
E-mail: f.fantuzzi@kent.ac.uk

Nanomaterials have garnered considerable attention owing to their exceptional properties and potential applications across diverse fields, such as electronics, medicine, energy, and environmental science. To design and optimize nanomaterials for specific applications, an atomistic understanding of their behavior at the nanoscale is imperative. With such understanding, the properties and performance of nanomaterials can be tailored to meet specific needs, and new materials with novel functionalities can be developed. In this work, two different processes at the nanoscale are computationally investigated using distinct approaches: i) the collision-induced structural transformation of graphene nanoflakes [1] into carbon nanotubes using reactive molecular dynamics simulations, and ii) the formation of distinct classes of lithium-fluoride nanotubes using Born-Oppenheimer molecular dynamics and periodic density functional theory (DFT) calculations [2,3]. In the first approach, we use the MBN Explorer computational package [4]. Molecular collisions between a C<sub>60</sub> fullerene and a graphene nanoflake are simulated with varying collision energies and impact angles. The results reveal that collision-mediated transformation of graphene nanoflakes into carbon nanotubes can happen under given collision conditions. The process is dependent on the projectile angle incidence and the relative masses of the nanoflake and the projectile. In the second approach, Born-Oppenheimer molecular dynamics and periodic density functional theory (DFT) calculations are used to study the mechanism of formation of stable lithium fluoride nanotubes with different cross-sections. Various transient species, such as nanowires, nanorings, nanosheets, and nanopolyhedra, are identified. The results suggest that template-driven synthetic techniques could be combined with stochastic methods to efficiently generate lithium fluoride nanotubes. Furthermore, the structural and electronic properties of prototypical lithium fluoride nanotubes featuring armchair, zigzag, and square sheet configurations are also investigated using DFT. The results indicate that the zigzag nanotubes can be formed from the more stable square sheet structures by applying a positive axial strain, and all nanotubes investigated are insulators with high stability and promising technological applications.

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## Imaging neuromorphic dynamics of percolating nanocluster networks

Miloš Baljuzović<sup>1</sup>, James E. McCormack<sup>1</sup>, Ella Kitching<sup>2</sup>, Malcolm Dearg<sup>2,3</sup>, Mohsen Danaie<sup>3</sup>, Yubiao Niu<sup>1</sup>, Thomas Slater<sup>2,3</sup>, Thierry Maffei<sup>1</sup>, Richard E. Palmer<sup>1</sup>, Richard J. Cobley<sup>1</sup>

<sup>1</sup>Nanomaterials Lab, Faculty of Science and Engineering, Swansea University, Bay Campus, Fabian Way, Swansea, SA1 8EN, United Kingdom

<sup>2</sup>School of Chemistry, Cardiff University, Main Building, Park Place, Cardiff, CF10 3AT, United Kingdom

<sup>3</sup>Electron Physical Science Imaging Centre, Diamond Light Source Ltd., Oxfordshire, OX11 0DE, United Kingdom  
E-mail: milos.baljuzovic@swansea.ac.uk

Scaling down the size of silicon-based devices to improve cost and performance has enabled some of the greatest achievements of humankind. However, this approach is coming to its ultimate limits imposed by reaching the dimensions where quantum size effects emerge. In order to address this challenge, novel materials and computational approaches are required. Brain-inspired computation, also called neuromorphic computing, has the potential to overcome certain limitations of conventional silicon technology, offering a new generation of faster, low-power computing [1,2]. Percolating networks of atomic clusters display fascinating physics such as voltage switching behaviour as found in the brain; nevertheless, the understanding of the origins of these effects is to date immature. In the context of growing interest in percolating nanocluster networks, no-one has yet demonstrated the ability to controllably fabricate nanocluster metal networks together with the experimental capability to directly study, atomistically, the electrical behavior of metallic 'synapses' – and thus unravel how the nanoscale conducting pathways form or change with applied stimulus [3-8].

In this contribution, I will present our recent results obtained using a state-of-the-art aberration-corrected scanning transmission electron microscopy, equipped with an in-situ sample electrical measurement stage, which allow us to image the percolating nanocluster networks with atomic resolution while operating these networks via the application of variable bias. Our results provide unprecedented insight into the real-time correlations between electrical switching and clear structural changes, revealing the emergent neuromorphic dynamics of the percolating nanocluster networks under operating conditions.

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## Multiscale modeling of Au-C nanostructured systems: Nanoparticle shapes and neuromorphic dynamics

Theodoros Pavloudis<sup>1,2</sup>

<sup>1</sup>Department of Physics, Aristotle University of Thessaloniki,  
GR-54124 Thessaloniki, Greece

<sup>2</sup>Nanomaterials Lab, Mechanical Engineering, Swansea University,  
Bay Campus, Fabian Way, Swansea, SA1 8EN, UK  
E-mail: tpavlo@auth.gr

The unique physical and chemical properties of carbon-based materials -graphene being the primary example- and of nanoparticles (NPs) can be further enhanced by combining the two in hybrid nanostructures. Indeed, NP-graphene composites show promise for electrochemical, energy, sensing and bio applications and as catalysts for various reactions. Amongst NPs, Au is attractive for most applications due to its stability, biocompatibility and catalytic activity, and has been a well-established model material in nanocluster science [1].

Focusing on this combination of materials, we firstly demonstrate the stabilization of two-dimensional (2D) Au rafts containing up to ~60 atoms on amorphous carbon, fabricated by sputtering of atoms and imaged by aberration-corrected scanning transmission electron microscopy. These rafts deviate from the established cluster transition from 2D to 3D structural motifs predicted theoretically for free clusters, which was expected to occur in the region of 10 – 14 atoms. We validate our experimental findings by performing explicit *ab initio* calculations of Au<sub>n</sub> (n=3-147) clusters on graphene and reveal the role of cluster-surface interactions in the stabilization of the metastable Au cluster rafts on graphene. The transition from equilibrium 2D to 3D structures is delayed to n=19, while metastable 2D rafts compete with 3D structures for up to n=60. Since the catalytic activity of supported nanoclusters depends on their structure, the results are relevant to the catalytic performance of nanocluster-based catalysts.

Next, we investigate atomic cluster-based networks, which represent a promising architecture for the realization of neuromorphic computing systems and may overcome some of the limitations of the current computing paradigm [2]. The formation and breakage of synapses between the clusters are of utmost importance for the functioning of these computing systems. We present a molecular dynamics simulation, at elevated temperatures, of synapse (bridge) formation, and thermal breaking processes, between 2.8 nanometer-sized Au<sub>1415</sub> clusters deposited on a carbon substrate, a model system. Crucially, we find that the bridge formation process is driven by the diffusion of gold atoms along the substrate however small the gap between the clusters themselves. The complementary simulations of the bridge breaking process reveal the existence of a threshold bias voltage to activate bridge rupture via Joule heating. These results provide an atomistic-level understanding of the fundamental dynamical processes occurring in neuromorphic cluster arrays.

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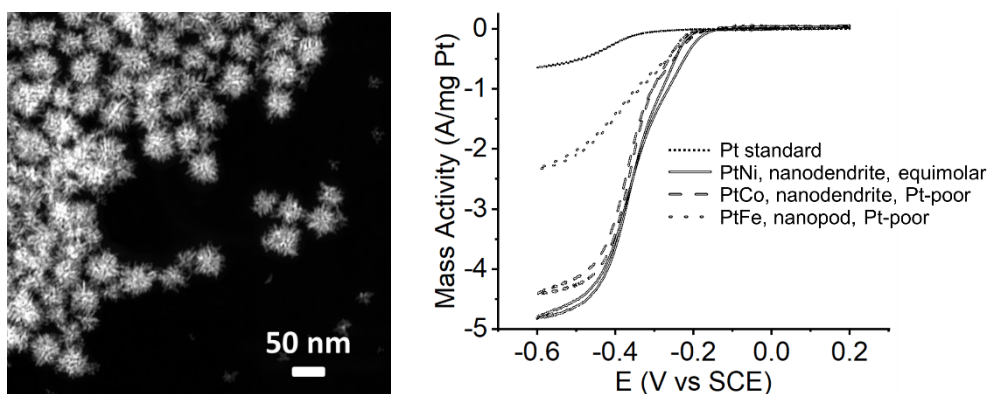
## Dual control of morphology and composition in heterobimetallic catalysts for oxygen reduction

Andrew E. H. Wheatley, Siyi Ming, Samuel J. Cobb, Erwin Reisner

Yusuf Hamied Department of Chemistry, University of Cambridge,  
Lensfield Road, Cambridge, CB2 1EW, UK  
E-mail: aehw2@cam.ac.uk

Metal nanoparticles with branched morphologies (e.g. nanopods) attract interest because of the link between catalytic activity and high surface-area-to-volume ratios. These are enhanced by branching, which exposes more active sites and enables the use of lower catalyst loadings [1]. Additionally, it has been shown that the efficacy of Pt for promoting the oxygen reduction reaction (ORR) is improved by forming intermixed PtM (M = Fe/Ni/Co) nanopods [2] or PtFe-Fe<sub>3</sub>O<sub>4</sub> nanopod-nanocube dimers [3]. Choice of parameters like particle surface capping agent and temperature have been used to offer insights into nanopod formation. More recently, even more complex nanodendrites have been reported [4], though their synthesis has been rather empirical. In both cases, the importance of varying morphology while maintaining bimetallic composition or vice versa have been recognized. Yet these remain elusive targets.

We report the one-pot combination of Pt with M under a range of conditions, yielding bimetallic nanoparticles whose construction sheds new light on nanopod and/or nanodendrite formation. Systematic modulation of experimental conditions allows the reduction of metal precursors to initially give nanopods. We show that morphology control can be maintained while composition is varied. The conditions are then identified for promoting the collision-based branching of nanopod arms and the selective growth of compositionally controlled nanodendrites. This level of synthetic control has enabled the systematic formation of both nanopods and nanodendrites with Pt-rich, equimolar and Pt-poor compositions. Following immobilization, these have been tested against industry standard Pt in ORR electrocatalysis under alkaline conditions (Figure 1). Onset potentials of the new branched catalysts are compelling compared with that of the standard, and they outperform it significantly in terms of current produced normalized for Pt content.



**Figure 1:** Representative STEM HAADF imaging of equimolar PtNi nanodendrites (left). Mass activity of selected PtM electrocatalysts versus Pt standard (right).

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## The challenge of the spontelectric state

D. Field, A.M.Cassidy

Center for Interstellar Catalysis, Physics and Astronomy, Aarhus University,  
Ny Munkegade, Dk 8000 C, Aarhus, Denmark  
E-mail: dfield@phys.au.dk, amc@phys.au.dk

The condensation of polar molecules onto a cold surface forms films supporting a large spontaneous electric field, a phenomenon dubbed the ‘spontelectric effect’. The challenge is to understand the physical mechanism through which the spontelectric effect arises. The spontaneous field may be in excess of  $10^8 \text{ Vm}^{-1}$ , a value strongly dependent on the temperature of the surface [1-3]. This is a many body effect, occurring in the bulk and requiring films of  $>5$  to 10 monolayers (ML). The physical nature of the surface is immaterial and the effect may be observed unchanged for surfaces as disparate as magnesium fluoride, gold or solid xenon.

By some undiscovered means, gas phase molecules settle into a configuration in which there is residual molecular orientation, as they become a part of the growing film. The film is spontaneously polarized, with an internal electric field. We ask, what is the aspect of the dynamics of this non-ergodic system forcing it into a local stable minimum and preventing the establishment of thermodynamic equilibrium? Can we pinpoint the driving force which leads to this unexpected phenomenon?

The present status of our understanding of the transition from the disordered gas phase to the solid state, with partial dipole ordering, is as follows. (i) we have developed a parameterized model which can reproduce the observed variation of the spontelectric field and consequent Stark shifts in infrared and VUV absorption energies, with deposition temperature, for a range of polar species. The model includes a stiffness factor for the mutual rotation of polar species, which may be the key [1]. (ii) an elegant molecular dynamics calculation [4] was able to reproduce the variation of the degree of orientation of *cis*-methyl formate with deposition temperature - although poorly the absolute degrees of orientation. (iii) molecular dynamics simulations show the development of spontaneous fields in porous amorphous solid water, though poorly the observed absolute values [5]. In addition there is a hand-waving explanation attributing the non-ergodicity to fluctuations in molecular orientation [6]. This latter has the advantage of contributing some sort of physical picture, whereas the parameterized model, (i), merely assumes the presence of orientation and (ii) and (iii) do not allow you to assign any specific mechanism to the formation of the spontelectric state and give little insight into its cause.

Can MesoBioNano Explorer (MBN Explorer), or some related molecular dynamics package, do the trick and reveal how dipole orientation spontaneously arises in vacuum-deposited thin films? This is a fundamental phenomenon, which cries out for an explanation. Is anyone here game to trying this?

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## Reversible chemisorption of gases on nanostructures for gas sensing

Vincenzo Guidi<sup>1</sup>, Barbara Fabbri<sup>1</sup>, Elena Spagnoli<sup>1</sup>, Francesco Tralli<sup>1</sup>, Arianna Rossi<sup>1</sup>,  
Andrey V. Solov'yov<sup>2</sup>

<sup>1</sup>Department of Physics and Earth Sciences, University of Ferrara, Via Saragat 1/C, 44123, Ferrara, Italy

<sup>2</sup> MBN Research Center, Altenhöferallee 3, 60438 Frankfurt am Main, Germany

E-mail: vincenzo.guidi@unife.it

Chemoresistive gas sensors are currently supplied by several companies and used in a wide range of applications, including industrial emission control, household security, vehicle emission control, environmental monitoring and agricultural and biomedical applications [1]. Gas sensors have attracted the attention of many users and scientists due to their low cost, flexibility of production, ease of use, long term stability and large number of detectable gases. The receptor element typically consists of a sensitive semiconducting metal oxide (SMOX) nanostructured layer deposited on the top of a substrate equipped with electrodes used to measure the electrical signal. Moreover, the SMOX film is commonly thermo-activated by means of a heater. Chemoresistive gas sensors belong to the class of chemical sensors and the signals arise from the change in the electrical properties of the semiconducting film induced by reversible redox reactions of the gaseous analyte over its surface. The main parameters controlling the sensitivity and selectivity of a SMOX-based sensor are gas diffusion along the meso/micro-porous sensing layer, gas adsorption equilibrium and material reactivity.

Nanostructured SMOXs have been extensively researched since in the late 1980s [1], which has led to a comprehensive understanding of these nanomaterials and finally allowed to rely on consolidated methodologies for their control. To date, lack of knowledge still persists on the mechanisms of gas reaction occurring at the surface of the nanostructures. Indeed, this information is fundamental for fine-tuning of material characteristics for any specific gas sensing applications.

To this aim, Diffuse Reflectance Infrared Fourier Transform (DRIFT)-spectroscopy is one of the most effective and advanced methods to examine the composition of rough-surfaced solid samples such as nanostructured semiconducting films. Then, an *operando* approach has been used to combine the electrical characterization of sensors in conditions for real applications together with DRIFT spectroscopy for the investigation of gas-surface reactions. In this contribution, we present state of the art research on this topic.

Very often, reaction dynamics proceeds too fast to be determined by DRIFT, resulting in limited information. Indeed, simulations by molecular dynamics including chemical reactions in heterogeneous phase, would be an important tool to support experimental analyses. Here we propose the usage of MesoBioNano (MBN) Science to study the dynamics of physical or chemical adsorption of gaseous molecules on a SMOX surface [2]. Preliminary results will be shown.

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**XRD and PAS investigation of crystal lattice defects induced in Zr  
by low energy deuterons**

K. Czerski<sup>2</sup>, A.Kowalska<sup>1</sup>, P. Horodek<sup>3</sup>, K. Siemek<sup>3</sup>, J. Słowik<sup>4</sup>, J. Baranowska<sup>4</sup>, M. Kaczmarowski<sup>2</sup>,  
R. Dubey<sup>2</sup>, M. Valat<sup>2</sup>, N. Targosz-Słęczka<sup>2</sup>

<sup>1</sup>Institute of Mathematics, Physics and Chemistry, Maritime University of Szczecin,  
Wały Chrobrego 1-2, 70-500, Szczecin, Poland  
E-mail: a.kowalska@pm.szczecin.pl

<sup>2</sup> Institute of Physics, University of Szczecin,  
Wielkopolska 15, 70-451, Szczecin, Poland  
E-mail: konrad.czerski@usz.edu.pl; mateusz.kaczmarowski@usz.edu.pl;  
mathieu.valat@usz.edu.pl; rakesh.dubey@usz.edu.pl; natalia.targosz-sleczka@usz.edu.pl;

<sup>3</sup> Institute of Nuclear Physics, Polish Academy of Science,  
Radzikowskiego 152, 31-342, Kraków, Poland

E-mail: pawel.horodek@ifj.edu.pl ; krzysztof.siemek@ifj.edu.pl

<sup>4</sup> Materials Engineering, West Pomeranian University of Technology,  
Piastów 19, 70-310 Szczecin, Poland

E-mail: justyna.slowik@zut.edu.pl ; jolanta.baranowska@zut.edu.pl

Recent studies of the deuteron-deuteron nuclear reactions in metallic targets, at projectile energies far below the Coulomb barrier, show a significant enhancement of cross sections due to the electron screening effect and the threshold resonance contribution. Both effects are sensitive to the local crystal structure and crystal lattice defects of the target material. This has a strong influence on both hydrogen diffusion and the effective electron mass. The latter determines the strength of the local electron screening effect [1] and can change the deuteron-deuteron reaction rates at thermal energies by many orders of magnitude [2].

The  ${}^2\text{H}(d,p){}^3\text{H}$  reaction taking place in Zr target has been studied using the unique accelerator system with ultra-high vacuum, installed in the eLBRUS laboratory at the University of Szczecin [3]. The metallic samples exposed to various conditions and energies of deuteron beams are then investigated by means of the X-ray diffraction (XRD) and positron annihilation spectroscopy (PAS) [4]. Whereas the first method delivers information about changes of crystal lattice parameters and possible production of hydrides [5,6] accompanying the formation of dislocations that are produced during irradiation of the samples, the second one can determine the depth distribution of crystal defects, being especially sensitive for vacancies. Both investigation methods show structural changes of the metallic samples. The target structure modifications at the surface of the samples could be also confirmed by the scanning electron microscopy (SEM). The presented diagnostic methods will be applied in the future studies to correlate the number of crystal defects and changes of crystallographic parameters with the increase of the deuteron-deuteron nuclear reaction rates.

The study is part of the CleanHME project. This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 951974.

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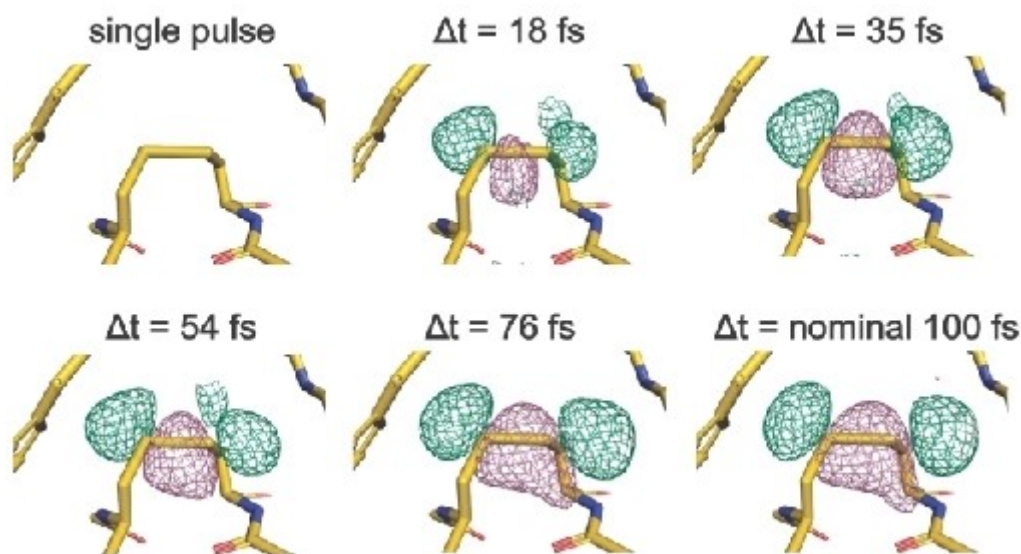
## Femtosecond dissociation of disulfide bridges within X-ray irradiated thaumatin crystal

Beata Ziaja-Motyka<sup>1,2</sup>

<sup>1</sup>Center for Free-Electron-Laser Science CFEL, Deutsches Elektronen Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany

<sup>2</sup> Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 85, 22607 Hamburg  
E-mail: ziaja@mail.desy.de

X-ray free-electron lasers (XFELs) enable crystallographic structure determination beyond the limitations imposed upon synchrotron measurements by radiation damage. The need for very short XFEL pulses is relieved through gating of Bragg diffraction by loss of crystalline order as damage progresses, but not if ionization events are spatially non-uniform due to underlying elemental distributions, as in biological samples. Indeed, correlated movements of iron and sulfur ions were observed in XFEL-irradiated ferredoxin microcrystals using unusually long pulses of 80 fs. Here, we report a femtosecond time-resolved X-ray pump/X-ray probe experiment on protein nanocrystals. We observe changes in the protein backbone and aromatic residues as well as disulfide bridges. Simulations show that the latter’s correlated structural dynamics are much slower than expected for the predicted high atomic charge states due to significant impact of ion caging and plasma electron screening. This indicates that dense-environment effects can strongly affect local radiation damage-induced structural dynamics [1].



**Figure 1:** Difference electron density for the Cys56-Cys66 disulfide bond in thaumatin as a function of X-ray pump - X-ray probe delay.

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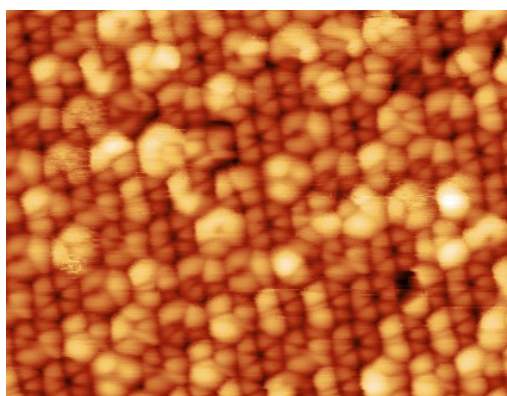
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## Imaging interstellar dust grain model surfaces and reaction products with atomic resolution

Liv Hornekær, Frederik D. Simonsen, Signe Kyrkjebø, Laura Slumstrup, Richard Balog, and John Thrower

Center for Interstellar Catalysis, Dept. Physics and Astronomy  
Aarhus University  
Ny Munkegade 120, DK-8000, Aarhus C, Denmark  
E-mail: liv@phys.au.dk

Interstellar space is home to surprisingly complex chemistry. In spite of the low temperatures and pressures more than 250 different molecules have so far been detected. Catalytic reactions on dust grain surfaces are expected to play a dominant role in interstellar chemistry. Such heterogenous catalytic reactions are highly dependent on the specifics of the catalytic surface. The elemental composition, defects, nanostructure, porosity, ice coatings and thick icy layers all impact heavily on reactivity. Scanning tunneling microscopy (STM) allow us to image surface structures and adsorbate molecules at the atomic level. Such measurements allow us to detect reaction products with single molecule detection sensitivity and to study the structure of low temperature icy clusters forming on surfaces of interstellar relevance. Here we present results on water ice cluster formation at temperatures down to 12 K and on imaging reaction products from PAH hydrogenation reactions [1-2].



**Figure 1:** Scanning tunneling microscopy (STM) image of superhydrogenated Coronene molecules on a graphite surface obtained at 5 K.

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## Charged particle impact experiments on astrophysical ice analogues

Péter Herczku<sup>1</sup>, Béla Sulik<sup>1</sup>, Duncan V. Mifsud<sup>1,2</sup>, Zoltán Juhász<sup>1</sup>, Sándor T. S. Kovács<sup>1</sup>, Richard Rácz<sup>1</sup>, Sándor Biri<sup>1</sup>, Rahul K. Kushwaha<sup>1</sup>, Sergio Ioppolo<sup>3,4</sup>, Nigel J. Mason<sup>1,2</sup>, Alejandra Traspas Muiña<sup>4</sup>, Zuzana Kaňuchová<sup>5</sup>, Robert W. McCullough<sup>6</sup>

<sup>1</sup>Institute for Nuclear Research (ATOMKI),  
Bem sqr 18/C, H-4026, Debrecen, Hungary

<sup>2</sup>Centre for Astrophysics and Planetary Science, School of Physics and Astronomy, University of Kent,  
Canterbury CT2 7NH, United Kingdom

<sup>3</sup>Centre for Interstellar Catalysis (InterCat), University of Aarhus, Aarhus 8000, Denmark

<sup>4</sup>School of Electronic Engineering and Computer Science, Queen Mary University of London  
London E1 4NS, United Kingdom

<sup>5</sup>Astronomical Institute, Slovak Academy of Sciences  
SK-059 60 Tatranská Lomnica, Slovakia

<sup>6</sup>Department of Physics and Astronomy, School of Mathematics and Physics, Queen’s University Belfast  
Belfast BT7 1NN, United Kingdom  
E-mail: herczku.peter@atomki.hu

In the interstellar medium the chemistry of simple molecules may result in the production of complex molecules. If the partners in the chemical reaction are organic molecules, the daughter molecule can be a complex organic molecule (COM). Through different reaction routes, the building blocks of life can be built up from COMs. To understand how life evolves, it is necessary to probe the chemistry of simple and complex molecules under conditions that simulate interstellar environments. In dense molecular cores, the molecules are exposed to ionizing radiation, which may act as an important driver of molecular destruction and synthesis.

At ATOMKI in Debrecen, we have two end-stations at the beamlines of two different accelerators, dedicated to exploring the radiative processing of complex molecular ice analogues similar that which can be found in the interstellar medium and the outer Solar System. Through the introduction of both set-ups (Ice Chamber for Astrophysics/Astrochemistry (ICA) [1] and the Atomki-Queens University Ice chamber for Laboratory Astrochemistry (AQUILA)), we would like to present our recent results achieved so far.

We carried out systematic and comparative investigations on CH<sub>4</sub>:H<sub>2</sub>O ice mixtures upon irradiation by 1 MeV H<sup>+</sup> and 2 keV electrons [2]. Our results demonstrate that irradiations result in the formation of various new products, including both simple and complex daughter molecules. The comparison of different irradiation regimes has also revealed that the proton irradiation is more productive in generating radiolytic daughter molecules compared to electron irradiation, despite the lower radiation dose. These results are important in the context of radiation chemistry occurring within the molecular cores of dense interstellar clouds and outer Solar System objects.

We have also investigated the implantation of sulphur ions into CO<sub>2</sub> ice [3]. In our Solar System, sulphur chemistry is best associated with Galilean moon system of Jupiter. The most volcanically active moon, Io, emits large quantities of sulphurous molecules. These molecules can be dissociated and ionized in the Jovian magnetosphere and subsequently interact with the icy surfaces of other Galilean moons. The observation of SO<sub>2</sub> ice in the surface of Europa has created a debate within the community regarding the source of its sulphur atom. We have demonstrated that the implantation of sulphur ions into CO<sub>2</sub> analogous to those that may be found on the surface of Europa does not likely yield SO<sub>2</sub>, as this process is temperature-dependent with lesser quantities of sulphurous molecules formed at higher temperatures.

In the talk we would like to present the capabilities of both set-ups and the further plans on possible experiments and developments.

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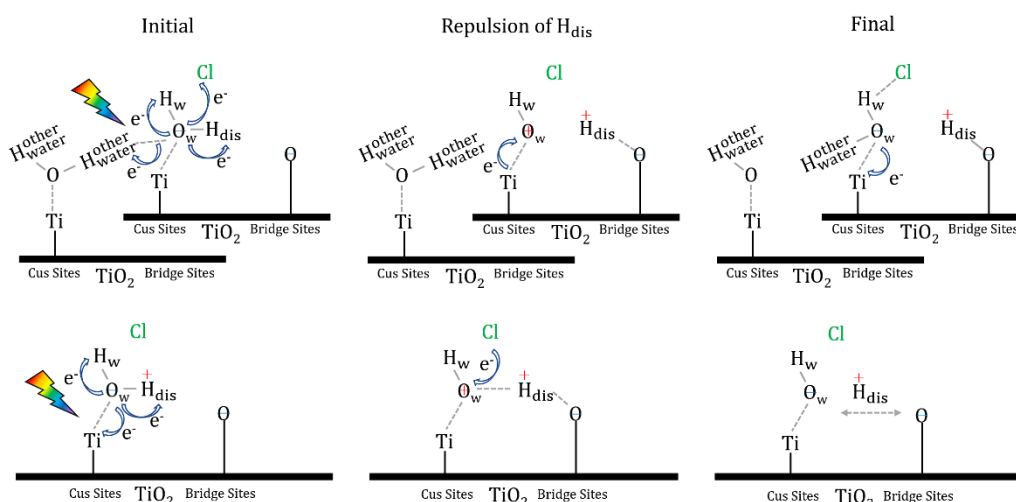
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## Nonadiabatic molecular dynamics simulations of chlorine behavior at nanostructured $\text{TiO}_2(110)$ /water interface

Sergei Piskunov, Yin-Pai Lin, Dmitry Bocharov, Inta Isakoviča, Ilja Markins

Institute of Solid State Physics, University of Latvia, 8 Kengaraga str., LV-1063 Riga, Latvia  
E-mail: piskunov@cfi.lu.lv

Chloride is a prevalent ion in seawater, which is more abundant than freshwater. The complexity in water dissociation on the rutile  $\text{TiO}_2$  nanofilm has been described by the lack of  $\text{H}_2\text{O}$  adsorbate states near the valence band maximum (VBM) edge. This occurs when the excitation energy is around the band gap energy of  $\text{TiO}_2$ . It is of interest to investigate whether the additional chlorine can be beneficial for water dissociation. In this study, we constructed models of chlorine adatoms on the rutile  $\text{TiO}_2(110)$ /water interface using ab initio approaches. We calculated time-dependent spatial charges, bond-lengths of water molecules, and Hirshfeld charges using real-time time-dependent density functional theory and the Ehrenfest dynamics theory to investigate the nonadiabatic dynamics of water dissociation taking into account the excited states. Our study suggests two photoinduced water-splitting pathways related to chlorine and analyzes the photogenerated hole along the reactions.



**Figure 1:** Predicted scenario of water molecule dissociation at  $\text{TiO}_2(110)$  in the presence of chlorine.

The first step of water dissociation relies on the localized competition of charges transferred between the dissociated water molecule and the adsorption site of  $\text{TiO}_2$ , which transforms the water into hydroxyl and hydrogen by photoinduced driving force. The first steps for water-splitting, which could be accomplished by the thermal equilibrium from the temperature and atomic environment, as well as the localized charge transferring from the photoexcitation, have been reported via modeling the  $\text{Cl}/\text{H}_2\text{O}/\text{slab}$  surface models in this study. The chlorine at the surface with  $\text{H}_2\text{O}$  adsorbate could trigger the dehydrogenation of a water molecule from the thermal effect and photoexcitation (Fig. 1). Combining photoexcitation and thermal dynamics is a significant challenge due to the crossing time scales and different governing equations, which also raises the question of whether photoinduced dissociations could still occur from femtoseconds to picoseconds. Additionally, constructing more realistic atomic structures is another challenge to enhance the value of the computational results. In this work, we consider atomic motions and electronic structures, as well as photoexcitation and thermal dynamics simultaneously, by adding extra chlorine on the water/ $\text{TiO}_2$  interface. This helps guide the design inspirations for photocatalytic systems and their applications in photoinduced water-splitting.

## Electrochemical nanotechnology: 3D printing of metals at the nanoscale

Dmitry Momotenko<sup>1</sup>, J. Hengsteler<sup>2</sup>, B. Mandal<sup>2</sup>, Genevieve Lau<sup>3</sup>, C. van Nisselroy<sup>2</sup>, T. Zambelli<sup>2</sup>, K. Kanés<sup>1</sup>, L. Khasanova<sup>1</sup>

<sup>1</sup>Department of Chemistry, Carl von Ossietzky University of Oldenburg,  
Carl von Ossietzky Strasse 9-11, 26129, Oldenburg, Germany

<sup>2</sup>Institute for Biomedical Engineering, ETH Zürich,  
Gloriastrasse 35, CH-8092, Zürich, Switzerland

<sup>3</sup>School of Physical and Mathematical Sciences, Division of Chemistry and Biological Chemistry, Nanyang Technological University,  
637371, Singapore

E-mail: Dmitry.momotenko@uol.de

Additive manufacturing, also commonly known as 3D printing, is rapidly becoming a part of our everyday life: from DIY use by hobbyists to industrial manufacturing, 3D printing is experiencing a booming success. The technologies advance quickly with faster print rates, broader choice of materials and a constantly increasing accuracy and printing resolution. Impressively, state-of-the-art techniques take the printed feature sizes to the extreme: multiphoton optical stereolithography and focused electron or ion beams are now capable to produce objects with nanoscale resolution. Although at the cutting edge to printing finest details, these advanced manufacturing methods lack the capacity to process dense and pure electrical conductors – materials very much needed to push the limits of the technologies of the future – sensors, energy storage devices, logical gates and memory interfaces.

Electrochemical methods, which have an advantage to process a wider range of materials – conductors and semiconductors, bulk materials and colloids, at a first glance, have little to do with additive manufacturing. For example, electrodeposition, a well-established approach traditionally used to produce metallic coatings or thin films, is often integrated in microfabrication process but is limited to planar two-dimensional designs. However, when combined with state-of-the-art nanoelectrochemical approaches, electrodeposition can be taken into a three-dimensional realm, where it can be used to produce complex structures with micro- and nanoscale dimensions [1]. The key to achieve this is nanoscale confinement of precursor delivery that is combined with layer-by-layer additive processing. Liquid manipulation by pressure driven flow through nanoscale cantilevers [2], intermittent meniscus formation using droplet cells [3], or droplet generation at high voltages – a variety of nanoelectrochemical techniques can be used to fabricate metallic structures with various morphologies. The recent advances in these technologies including instrumental aspects, performance metrics such as resolution and print rates, as well as some materials characteristics are highlighted here.



**Figure 1:** Artistic representation of an electrochemical 3D printing process in electrolyte meniscus at the tip of a glass nanopipette nozzle.

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**Playing with the photophysics of atomically precise nanoclusters:  
From photo-thermal to photodynamic effects**

Rodolphe Antoine

Institut lumière matière, UMR5306, Université Claude Bernard Lyon1-CNRS,  
Univ. Lyon 69622, Villeurbanne cedex, France.

E-mail: rodolphe.antoine@univ-lyon1.fr

Ligand protected metal nanoclusters (NCs) are an emerging class of quantum materials connecting the gap between atoms and bulk metallic materials [1]. Owing to their unique electrical, optical and other spectroscopic properties such as luminescence, they are very important in various applications such as sensing and bio-imaging [2-5]. Concerning optical properties, strongly emissive nanoclusters are highly desirable. On one hand, radiative relaxation pathways (occurring from surface, core and triplet states) lead to a rich and color-tunable photoluminescence (PL), in particular for NIR imaging. On the other hand, non-radiative pathways promote interaction of nanoclusters with their surrounding media (liquid) and thus inducing heating, leading to nanobubbles formations enhancing acoustic waves, particularly appealing for photoacoustic imaging. Beyond imaging capabilities (both by photoacoustic and NIR fluorescence techniques), such photophysical process may promote interesting processes for therapy. Indeed, inter-system crossing opening for triplet states populations can be the basis for reactive oxygen species generation (key ingredient for photodynamic therapy) [6]. Of course the non-radiative pathway inducing heating can be used also for therapy actions, known as photothermal therapy [7].

In this lecture, I will describe some strategies aiming at playing with the photophysical properties of atomically precise gold nanoclusters, from photo-thermal to photodynamic effects.

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**Using superatomic metal-chalcogenide clusters and charge transfer ligands for nano p- n- junctions with tunable band gaps and band alignment, light harvesting and CO<sub>2</sub> conversion**

S.N. Khanna, A.C. Reber, T. Sengupta

Physics Department, Virginia Commonwealth University, Richmond VA 23284-2000, USA  
E-mail: snkhanna@vcu.edu

Organic ligands attached to the surfaces of clusters and nanoparticles are generally considered to be inert passive coatings. I will first present our results that show that ligands can strongly affect redox properties of clusters. Attaching phosphine ligands to simple metal, noble metal, semiconducting, metal-oxide, and metal-chalcogen clusters is shown to severely reduce ionization energies in all classes of clusters. Several of the simple and noble metal-ligated clusters are transformed into super donors with ionization energies nearly half that of cesium atoms and extremely low second and third ionization energies. The reduction in ionization energy can be split into initial and final state effects. The initial state effect derives in part from the surface dipole but primarily through the formation of bonding/antibonding orbitals that shifts the highest occupied molecular orbital. The final state effect derives from the enhanced binding of the donor ligand to the charged cluster. An opposite effect is observed if the donor ligands are replaced by acceptor ligands including CO. Ligation is shown to be an outstanding strategy for the formation of multiple electron donors/acceptors. I will present experimental evidence confirming the theoretical predictions.

I will then describe how such a strategy can be used to develop a new class of p-n junctions. Traditional p-n junctions used for photovoltaics require an interface where a light induced electron-hole pair is separated by an electric field. Developing alternative strategies for forming strong internal electric fields for electron-hole pair separation offers the possibility for better performance. We demonstrate that fusing two superatomic clusters with donor/acceptor ligands on opposite sides of the cluster leads to such a strong internal electric field. In two fused metal-chalcogenide  $\text{Re}_6\text{S}_8\text{Cl}_2(\text{L})_4$  clusters with donor  $\text{PMe}_3$  ligands and acceptor CO ligands on the opposite sides of the fused clusters, the electronic levels undergo shifts analogous to band bending in traditional p-n junctions. The fused cluster has a large dipole moment, and an optical spectrum that strongly absorbs excitation above the HOMO-LUMO gap of the fused clusters, but is optically very weak for the lowest energy excitation that can lead to electron-hole pair recombination. This is because the electron is localized on the CO portion of the fused cluster, while the electron-hole pair is localized on the  $\text{PMe}_3$  side of the cluster. It is shown that the electronic states localized on each side of the cluster can be aligned/misaligned by applying a voltage in different directions, offering diode like characteristics.

I will finally discuss our recent efforts in using ligated metal-chalcogenide clusters as catalysts for CO<sub>2</sub> conversion into formic acid. In particular, I will discuss how the reaction rates could be controlled by the choice of ligands.



**Horizon Europe EIC-Pathfinder Project TECHNO-CLS:  
"Emerging technologies for crystal-based gamma-ray light sources"**

Andrei V. Korol and Andrey V. Solov'yov

MBN Research Center, Altenhöferallee 3, 60438 Frankfurt am Main, Germany  
E-mail: korol@mbnexplorer.com; solovyov@mbnresearch.com

TECHNO-CLS project aims at the breakthrough in technologies needed for designing and practical realisation of novel gamma-ray Light Sources (LS) operating at photon energies from ~100 keV up to GeV range that can be constructed through exposure of oriented crystals (linear, bent and periodically bent) to the beams of ultra-relativistic charged particles [1]. The TECHNO-CLS high-risk/high-gain science-towards-technology breakthrough research programme will address the physics of the processes accompanying the oriented crystal exposure to irradiation by the high-energy electron and positron beams at the atomistic level of detail needed for the realisation of the TECHNO-CLS goals [2-4].

A broad interdisciplinary, international collaboration has been created previously in the frame of FP7 and H2020 projects, which performed initial experimental tests to demonstrate the crystalline undulator (CU) idea, production and characterisation of periodically bent crystals and the related theory (see [2-4] and references therein). TECHNO-CLS aims to build the high-risk/high-gain science-towards-technology breakthrough research programme on these successful studies aiming at a practical realisation of the novel gamma-ray LSs such as crystalline channeling radiation emitters, crystalline synchrotron radiation emitters, crystalline undulators and others. Additionally, by means of a pre-bunched beam a CU LS has a potential to generate coherent superradiant radiation with wavelengths orders of magnitudes less than 1 Angstrom, i.e. within the range that cannot be reached in existing LSs based on magnetic undulators. Such LSs will have many applications in the basic sciences including nuclear and solid-state physics and the life sciences. Theoretical, computational, experimental and technological results obtained in the course of this project will pave a way for key technological developments of the LSs and their wide exploitation. The TECHNO-CLS international collaboration possesses all the necessary expertise to conduct successfully the outlined programme.

There will be presented the main goals and the current developments within the TECHNO-CLS project. Particular emphasis will be made on the recent theoretical advances in atomistic simulations of channeling and radiation processes in oriented crystals [2-6] which were achieved by means of the advanced software packages MBN Explorer [7] and MBN Studio [8] during the last years.

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**Development of a positron beamline for channeling experiments at MAMI**

W. Lauth, H. Backe, I. Beltschikow, P. Drexler, P. Klag, F. Stieler

Institut für Kernphysik, Johannes-Gutenberg-Universität, D-55099 Mainz, Germany

E-mail: Lauthw@uni-mainz.de

The Institute for Nuclear Physics of the University of Mainz operates the accelerator complex MAMI which supplies an electron beam with a maximum energy of 1.6 GeV and a beam current of up to 100  $\mu\text{A}$ . Outstanding qualities of MAMI is the continuous beam with an excellent beam quality of  $4\pi$  nm rad emittance, a very low energy spread of less than  $10^{-4}$ , as well as its extremely high reliability. All kind of channeling experiments require such a high-quality beam with a low divergence. Positrons, however, are more preferable because they have a significant longer de-channeling length. The aim of a new project is the preparation of high-quality positron beam using the MAMI accelerator.

Positrons will be created by pair conversion of bremsstrahlung, produced by the 855 MeV electron beam of MAMI in a 10  $\mu\text{m}$  thick tungsten converter target, and energy selected by an outside open electron beam-line bending magnet. A sector magnet bents back the beam. Magnetic focusing elements in between are designed to prepare in a well shielded chamber about 6 m away from the converter target a beam spot. At an accepted positron band width of 1 MeV, spots are expected vertically with an angular spread of 0.064 mrad and a size of 5.0 mm (FWHM), and horizontally with an angular spread of 0.64 mrad and a size of 7.7 mm (FWHM). A positron yield is expected of 13 per second at 1 nA electron beam current and 1 MeV positron energy band width.

First investigations on the yield and divergence of the positron beam in a subsection of the beam line are presented and compared with the results of calculations. Possible experiments with this positron beam line will be discussed.

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**Channeling radiation experiments with multi-GeV electron and positron beams:  
Recent results and future perspectives**

L. Bandiera

on behalf of the INFN STORM/OREO collaboration

Istituto Nazionale di Fisica Nucleare (INFN), Section of Ferrara,  
Via Saragat 1, 44122, Ferrara, Italy  
E-mail: bandiera@fe.infn.it

The work presented here has been devoted to the investigation of high-intense electromagnetic radiation generation through axial channeling of ultrarelativistic electrons and positrons in oriented crystals. A series of experiments was carried out within the INFN STORM project in two different laboratories, i.e., the DESY Test Beam Facility in Hamburg and the Super Proton Synchrotron (SPS) at CERN in Geneva.

Firstly, we present the results of an experiment conducted at the DESY TB with a 5.6 GeV electron beam and a crystalline tungsten radiator. The electron beam crossed the axially oriented W crystal with the emission of channeling radiation, characterized by a considerably larger amount of photons if compared to standard bremsstrahlung. Experimental data clearly highlight an increased production of photons and of radiated energy [1]. The presented work opens the way for a realistic design of an intense crystal-based positron source for future lepton colliders, e.g. FCC-ee, CLIC, ILC or CePC, in which the increased number of photons would result in an increased production of positrons, if compared with conventional  $e^+$  sources based on bremsstrahlung targets.

Then, the results of an experiment on axial channeling (also known as *stochastic deflection*) of 120 GeV electrons and positrons in a bent crystal carried out at the H4 extracted line of CERN SPS are presented [2]. In particular, we investigated the deflection efficiency under axial confinement of both positrons and electrons as a function of the crystal orientation. Indeed, this was the first experimental evidence of axial deflection of ultrarelativistic electrons and positrons (or in general leptons) in bent crystals. The investigation showed that stochastic deflection is efficient for deflection of both positively and negatively charged particles. We also measured the emitted electromagnetic radiation by the electrons interacting with the crystal via stochastic deflection; the energy-loss spectrum resulted to be harder and more intense than for the case of random orientation. The deflecting and radiative power of axial channeling in bent crystals can be then exploited for collimation devices for future linear colliders.

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### **Pulsed laser melting for crystals bending**

D. De Salvador<sup>1,2</sup>, F. Sgarbossa<sup>1,2</sup>, D. Valzani<sup>1,2</sup>, G. Maggioni<sup>1,2</sup>, C. Carraro<sup>1,2</sup>, S. Bertoldo<sup>1,2</sup>, D. Fontana<sup>1</sup>, E. Di Russo<sup>1,2</sup>, E. Napolitani<sup>1,2</sup>

<sup>1</sup> Dipartimento di Fisica e Astronomia, Università di Padova, Via Marzolo 8, I-35131 Padova, Italy

<sup>2</sup> National Institute for Nuclear Physics INFN, Laboratori Nazionali di Legnaro, Viale dell'Università 2, 35020 Legnaro, Italy

E-mail: [davide.desalvador@unipd.it](mailto:davide.desalvador@unipd.it)

The pulsed laser melting (PLM) process can be successfully used to modify the electronic and structural properties of monocrystalline semiconductor materials.

PLM is a dynamic out-of-equilibrium process consisting in a high-intensity pulsed UV laser beam that liquefies crystal surface for hundreds of nanometres in a few nanoseconds. Subsequently, during cooling, the crystal solidifies by epitaxy in a hundred nanoseconds. If the crystal surface is deposited with a controlled layer of heterogeneous atoms, these diffuse into the liquid phase and are then incorporated during regrowth. The result is the incorporation of dopant/alloying atoms in large quantities usually higher than that obtainable with equilibrium processes. This process shows great advantages in hyperdoping applications in nanoelectronics, photonics and detector production.

Within the Europe TECHNO-CLS project, we are investigating the potential of this technique to produce curved crystals to be used in the development of novel gamma-ray Light Sources (LS) operating at photon energies from ~100 keV up to GeV range that can be constructed through exposure of oriented crystals (linear, bent and periodically bent) to the beams of ultra relativistic charged particles. In particular, crystalline undulator are ideally perfect crystals having a homogeneous harmonic curvature. Ultra-relativistic beams (positrons or electrons) can be trapped along the channels formed by crystalline planes (channeling) and can be steered along an undulating trajectory due to the crystal periodic curvature. Such a device will emit brilliant and directional light due to constructive interference of light and relativistic space contractions.

In this communication we describe two aspects of our investigation. We studied how the incorporation of antimony can lead to the production of stressor layers over germanium crystals which induce a curvature of thin substrates. Among possible candidates Sb induce both structural and electronic lattice expansion inducing the higher specific strain by unit of concentration. We investigated Ge crystals with different orientations and different Sb concentration and laser annealing parameters (energy and number of pulses). The structure of the layer was studied by X-ray diffraction and the curvature by surface profilometry.

Furthermore, in view of the use of PLM as a technique to induce periodic curvatures we investigated, through finite element simulations, innovative patterning strategies of stressor layers to optimize the homogeneity and harmonicity of the curvature in the inner part of the crystal.

**Progress on dynamic structural lattice modulation of single crystals  
for CLS applications**

Konstantinos Kaleris<sup>1,2,\*</sup>, Evaggelos Kaselouris<sup>1,2</sup>, Manos Kaniolakis-Kaloudis<sup>1,2</sup>, Makis Bakarezos<sup>1,2</sup>, Vassilis Dimitriou<sup>1,2</sup>, Michael Tatarakis<sup>1,3</sup>, Nektarios A. Papadogiannis<sup>1,2,\*\*</sup>

<sup>1</sup>Institute for Plasma Physics and Lasers (IPPL), Hellenic Mediterranean University, Tria Monastiria, GR-74100 Rethymnon, Greece

<sup>2</sup>Physical Acoustics and Optoacoustics Laboratory, Department of Music Technology and Acoustics, Hellenic Mediterranean University, GR-74100 Rethymnon, Greece

<sup>3</sup>Department of Electronic Engineering, Hellenic Mediterranean University, 73133 Chalepa, Chania, Greece  
\*E-mail: [kkaleris@hmu.gr](mailto:kkaleris@hmu.gr)

\*\*E-mail: [npapadogiannis@hmu.gr](mailto:npapadogiannis@hmu.gr)

The development of Crystal-based Light Sources (CLS) for the generation of brilliant  $\gamma$ -ray sources by exposing properly prepared crystal lattices to ultra-relativistic charged particle beams is a promising emergent field that is expected to open up radically new possibilities in various technological and scientific fields [1-3]. Crystalline Undulators (CUs) have attracted interest due to their technological feasibility and wide range of diverse implementations [1-5]. Currently, charged particle undulation is achieved by using strong periodic magnetic fields, which are commonly produced by expensive and large magnets in setups called Free Electron Lasers (FELs), commonly housed in large laboratories [6].

CUs are novel devices that take advantage of the remarkably high electric fields present in crystal lattices to induce undulation in ultra-relativistic  $e^-/e^+$  or charged hadron beams. These electric fields can attain strengths of up to  $10^{10}$  V/cm, an equivalent of 3000 T, that are significantly larger than the maximum of 10 T magnetic fields found in typical magnet undulators [2]. In CUs, undulation is induced by sinusoidal-like modulation of the lattice geometry, which can be done either statically, via structural deformation methods such as periodic mechanical stress, grooving, epitaxially-grown superlattices [1,2,7,8], or dynamically, through e.g. the launch of acoustic waves inside the crystal [9]. In the latter case, the enforced sinusoidal-like modulation of the lattice planes can cause the charged particles to follow sinusoidal-like trajectories, resulting in the emission of  $\gamma$ -ray photons with energies of up to several tens of MeV [2].

In this work, we present the ongoing progress on the development of acoustic wave (AW) CUs. AW CUs are among the least studied  $\gamma$ -ray CLS due to the challenging technicalities in their design, which are mainly related to the difficulty in the accurate control and characterisation of proper acoustic waves inside crystalline materials. Nevertheless, AW CUs are very promising as they can lead to tunable devices regarding both the period and amplitude of the lattice modulation, which is crucial for the technology development, i.e. for experimental optimization, but also in the intended applications. Moreover, compared to static lattice modulation techniques, e.g. mechanical bending, AW CUs allow for a large number of undulation periods to be induced inside the crystal, which is expected to lead to an important increase in the intensity of the emitted undulation  $\gamma$ -ray spectral peaks, for the case of charged particle channeling. The mentioned difficulties and potential benefits of the successful development of AW CUs render the presented project a high-risk high-gain scientific venture.

More specifically, in this work novel AW CU schemes will be presented for the generation of longitudinal waves inside Silicon [9] and Germanium monocrystals based on a typical Acousto-Optic Modulator (AOM) design. AOMs are implemented in either standing or travelling wave designs. Here, it will be argued that under real experimental conditions for the generation of semi-coherent brilliant narrowband  $\gamma$ -rays, travelling wave designs exhibit significant advantages over standing wave implementations. For this purpose, two different excitation methods will be investigated, particularly the well-established piezoelectric acoustic wave excitation and the recently proposed [10] laser-based excitation with the use of thin metallic film photoacoustic transducers. Results from Finite Element Method (FEM) simulations for the evaluation of the dynamic lattice deformations induced in the different proposed schemes for the undulation of ultra-relativistic beams will also be presented and discussed.

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Accurate diagnostic schemes based on imaging laser interferometry and laser Bragg diffraction for the precise characterisation of the acoustic waves and crystal lattice modulation will also be discussed. Finally, future work and a roadmap for the construction, characterisation and actual evaluation of the AW CUs in particle accelerator facilities will be outlined.

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## Investigation of radiation emitted by sub-GeV electrons in oriented scintillator crystals

L. Bandiera<sup>2</sup>, N. Canale<sup>2</sup>, D. De Salvador<sup>5,6</sup>, V. Guidi<sup>1,2</sup>, P. Klag<sup>3</sup>, W. Lauth<sup>3</sup>,  
A. Mazzolari<sup>2</sup>, R. Negrello<sup>1</sup>, G. Paternò<sup>2</sup>, M. Romagnoni<sup>2</sup>, F. Sgarbossa<sup>5</sup>,  
M. Soldani<sup>1,2</sup>, A. Sytov<sup>2</sup>, V. V. Tikhomirov<sup>4</sup>

<sup>1</sup>Department of Physics and Earth Sciences, University of Ferrara, Via Saragat 1, 44122, Ferrara, Italy

<sup>2</sup>INFN Section of Ferrara, Via Saragat 1, 44122, Ferrara, Italy

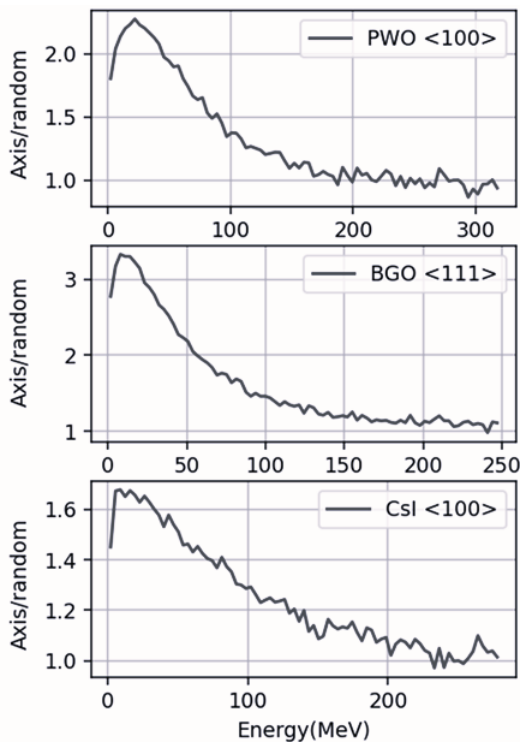
<sup>3</sup>Institut für Kernphysik der Universität Mainz, 55099, Mainz, Germany

<sup>4</sup>Institute for Nuclear Problems, Belarusian State University, Bobruiskaya 11, 220030, Minsk, Belarus

<sup>5</sup>Department of Physics, University of Padova, Via Marzolo 8, 35131, Padua, Italy

<sup>6</sup>INFN Laboratori Nazionali di Legnaro, Viale dell'Università 2, 35020, Legnaro, Italy

E-mail: riccardo.negrello@unife.it; laura.bandiera@unife.it



**Figure 1:** Axis vs random spectrum, for the different crystals, highlighting the enhancement in the emitted radiation

The presented research focuses on the study of coherent interactions of sub-GeV electrons with oriented scintillator crystals, resulting in an increase in the electromagnetic (EM) radiation generated. The experiment was conducted at the Mainz Mikrotron (MAMI), where PWO, BGO, and CsI crystals were mounted on a goniometer to set different orientations for the  $\langle 100 \rangle$ ,  $\langle 111 \rangle$ , and  $\langle 100 \rangle$  axes respectively. The chosen scintillating materials are commonly employed in nuclear, particle physics, applied and medical physics for detectors, EM calorimeters, etc. Here we show an increase in the emitted radiation when the beam is aligned to the crystal axis with respect to the random orientation (see Figure.1). In particular, the enhancement of EM processes has been investigated for the first time in BGO and CsI crystals.

The presented results are of interest for the realization of innovative detectors using oriented crystal scintillators, in which the EM processes are boosted when the beam direction is aligned with crystallographic directions. An elective application could be the development of ultra-compact and highly sensitive EM calorimeters for high energy and astroparticle physics. Further applications could be in high-performance gamma detectors for nuclear physics and medical imaging.

**Coupling X-ray beam induced current and X-ray diffraction imaging to characterize diamond plates used as semiconductor-based detectors**

F. Lafont<sup>1</sup>, M.L. Gallin-Martel<sup>2</sup>, D. Dauvergne<sup>2</sup>, P. Everaere<sup>2</sup>, R. Molle<sup>2</sup>, J. Baruchel<sup>1</sup>, T.N. Tran Caliste<sup>1</sup>

<sup>1</sup>European Synchrotron Radiation Facility, 71 avenue des Martyrs, 38000 Grenoble, France

<sup>2</sup>Laboratoire de Physique Subatomique et Cosmologie, 53 avenue des Martyrs, 38000 Grenoble, France  
E-mail: thu-nhi.tran-thi@esrf.fr

The demand for an accurate characterization of the electronic properties of semiconductors-based detectors, designed for physical and/or medical applications, is growing. This is particularly true for diamond-based detectors, which are very fast, radiation hardened and low noise. These features make them suitable candidates for a variety of applications. Indeed they can be used as beam monitors in current integration mode at very high particle rates, or in fast pulse detection mode for time stamp.

Based on previous experiments at the ESRF [1], we developed an X-Ray Beam Induced Current (XBIC) setup on BM05 at the ESRF aiming at characterizing the electronic properties of the commercially available diamonds. By recording 2-dimensionnal current maps we were able to evaluate the homogeneity of the detector response. Thanks to the availability of Bragg diffraction imaging [2] on the same beamline we also showed the correlations, on the percent level, between charge collection attenuation and structural defects such as growth sector boundaries or dislocations. The coupling of these two imaging techniques allows, for instance, showing that the large depletion in charge collection we observe on XBIC maps after proton irradiation do not correspond to structural defects. These coupled quantitative imaging tools (XBIC, X-ray diffraction imaging) can give clues for the optimization of semiconductor crystal growth and processes.

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## List of Participants

	<b>Surname</b>	<b>Name</b>	<b>Affiliation</b>	<b>E-mail</b>
1	Antoine	Rodolphe	Institut Lumière Matière, Université Lyon 1, Villeurbanne cedex, France	rodolphe.antoine@univ-lyon1.fr
2	Bald	Ilko	Institute of Chemistry, University of Potsdam, Potsdam, Germany	bald@uni-potsdam.de
3	Baljozović	Miloš	Nanomaterials Lab, Swansea University, United Kingdom	milos.baljozovic@swansea.ac.uk
4	Bandiera	Laura	Istituto Nazionale di Fisica Nucleare (INFN), Section of Ferrara, Italy	bandiera@fe.infn.it
5	Connerade	Jean-Patrick	Imperial College London, London, United Kingdom	jean-patrick@connerade.com
6	De Salvador	Davide	Dipartimento di Fisica e Astronomia, Università di Padova, Italy	davide.desalvador@unipd.it
7	Dickers	Matthew	School of Physics and Astronomy, University of Kent, Canterbury, UK	mdd27@kent.ac.uk
8	Dutta	Anushree	Institute of Chemistry, University of Potsdam, Potsdam, Germany	anushree.dutta@uni-potsdam.de
9	Ernst	Wolfgang	Institute of Experimental Physics, Graz University of Technology, Austria	wolfgang.ernst@tugraz.at
10	Falk	Martin	Institute of Biophysics of CAS, Brno, Czech Republic	falk@ibp.cz
11	Fantuzzi	Felipe	School of Chemistry and Forensic Science, University of Kent, UK	f.fantuzzi@kent.ac.uk
12	Field	David	Center for Interstellar Catalysis, Dept. of Physics and Astronomy, Aarhus University, Denmark	dfield@phys.au.dk
13	Gerhards	Luca	Institute of Physics, Carl-Von-Ossietzky University, Oldenburg, Germany	luca.gerhards@uni-oldenburg.de
14	Guidi	Vincenzo	Department of Physics and Earth Sciences, University of Ferrara, Italy	guidi@fe.infn.it
15	Hahn	Marc Benjamin	Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany	marc-benjamin.hahn@fu-berlin.de
16	Hallier	Dorothea	Fraunhofer Institute for Cell Therapy and Immunology, Potsdam, Germany	dorothea.hallier@izi-bb-extern.fraunhofer.de
17	Hausmann	Michael	Kirchhoff-Institute for Physics, Heidelberg University, Germany	hausmann@kip.uni-heidelberg.de
18	Herczku	Péter	Institute for Nuclear Research (ATOMKI), Debrecen, Hungary	herczku.peter@atomki.hu
19	Hornekær	Liv	Center for Interstellar Catalysis, Dept. of Physics and Astronomy, Aarhus University, Denmark	liv@phys.au.dk
20	Kaleris	Konstantinos	Institute for Plasma Physics & Lasers, Hellenic Mediterranean University Research Centre, Rethymno, Greece	kkaleris@hmu.gr
21	Khanna	Shiv	Virginia Commonwealth University, Richmond, VA, USA	snkhanna@vcu.edu
22	Klag	Pascal	Institute of Nuclear Physics, University of Mainz, Germany	pklag02@uni-mainz.de
23	Korol	Andrei	MBN Research Center, Frankfurt am Main, Germany	korol@mbnexplorer.com
24	Kowalska	Agata	Institute of Mathematics, Physics and Chemistry, Maritime University of Szczecin, Poland	a.kowalska@pm.szczecin.pl
25	Lauth	Werner	Institute for Nuclear Physics, Johannes Gutenberg-University, Mainz, Germany	Lauthw@uni-mainz.de
26	Marques	Telma	Campus Tecnológico e Nuclear, Instituto Superior Técnico, Bobadela, Portugal	telmasilva@ctn.tecnico.ulisboa.pt

27	Mason	Nigel	School of Physics and Astronomy, University of Kent, Canterbury, UK	N.J.Mason@kent.ac.uk
28	McElwee-White	Lisa	Department of Chemistry, University of Florida, USA	lmwhite@chem.ufl.edu
29	Momotenko	Dmitry	Department of Chemistry, Carl von Ossietzky University of Oldenburg, Germany	Dmitry.momotenko@uol.de
30	Negrello	Riccardo	Department of Physics and Earth Sciences, University of Ferrara, Italy	riccardo.negrello@unife.it
31	Pavloudis	Theodoros	Department of Physics, Aristotle University of Thessaloniki, Greece	tpavlo@auth.gr
32	Piskunov	Sergei	Institute of Solid State Physics, University of Latvia, Riga, Latvia	piskunov@cfi.lu.lv
33	Platonenko	Aleksandrs	Institute of Solid State Physics, University of Latvia, Riga, Latvia	alexander.platonenko@gmail.com
34	Schürmann	Robin	Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany	robin.schuermann@ptb.de
35	Shvalya	Vasyl	Department of Gaseous Electronics (F6), Jožef Stefan Institute, Ljubljana, Slovenia	Vasyl.Shvalya@ijs.si
36	Solov'yov	Andrey	MBN Research Center, Frankfurt am Main, Germany	solovyov@mbnresearch.com
37	Solov'yov	Ilia	Carl von Ossietzky University of Oldenburg, Oldenburg, Germany	ilia.solovyov@uni-oldenburg.de
38	Solovyeva	Irina	MBN Research Center, Frankfurt am Main, Germany	irina@mbnexplorer.com
39	Suraud	Eric	Université Paul Sabatier, Toulouse, France	suraud@irsamc.ups-tlse.fr
40	Tran Caliste	Thu Nhi	European Synchrotron Radiation Facility, Grenoble, France	thu-nhi.tran-thi@esrf.fr
41	Tsuchida	Hidetsugu	Quantum Science and Engineering Center, Kyoto University, Japan	tsuchida@nucleng.kyoto-u.ac.jp
42	Verkhovtsev	Alexey	MBN Research Center, Frankfurt am Main, Germany	verkhovtsev@mbnexplorer.com
43	Wheatley	Andrew	Dept. of Chemistry, University of Cambridge, United Kingdom	aehw2@cam.ac.uk
44	Ziaja-Motyka	Beata	Center for Free-Electron Laser Science, DESY, Hamburg, Germany	ziaja@mail.desy.de

**For notes**

**Monday, April 24**

08 <sup>00</sup> – 09 <sup>00</sup>	Participants registration
09 <sup>00</sup> – 09 <sup>10</sup>	<b>DySoN 2023 Opening</b> N.J. Mason, A.V. Solov'yov
09 <sup>10</sup> - 11 <sup>00</sup>	<i>Morning session I:</i> <i>Dynamics of systems on the nanoscale</i> <b>Andrey Solov'yov</b> <b>Ilko Bald</b> <b>Eric Suraud</b> <b>Hidetsugu Tsuchida</b>
11 <sup>00</sup> – 11 <sup>20</sup>	<b>Coffee break</b>
11 <sup>20</sup> - 13 <sup>10</sup>	<i>Morning session II:</i> <i>Structure and dynamics of biomolecular and biological systems</i> <b>Michael Hausmann</b> <b>Martin Falk</b> <b>Marc Benjamin Hahn</b> <b>Dorothea Hallier</b>
13 <sup>10</sup> – 14 <sup>30</sup>	<b>Lunch</b>
14 <sup>30</sup> - 16 <sup>10</sup>	<i>Afternoon session I:</i> <i>Structure and dynamics of molecules, clusters and nanoparticles</i> <b>Luca Gerhards</b> <b>Robin Schürmann</b> <b>Anushree Dutta</b> <b>Vasyl Shvalya</b>
16 <sup>10</sup> – 16 <sup>30</sup>	<b>Coffee break</b>
16 <sup>30</sup> – 18 <sup>30</sup>	<i>Afternoon session II:</i> <i>Clustering, self-organization, phase and morphological transitions on the nanoscale</i> <b>Wolfgang Ernst</b> <b>Felipe Fantuzzi</b> <b>Miloš Baljozović</b> <b>Theodoros Pavloudis</b>
19 <sup>30</sup> – 22 <sup>00</sup>	<b>Welcome reception</b>

**Tuesday, April 25**

9 <sup>00</sup> – 10 <sup>50</sup>	<i>Morning session I:</i> <i>Nanostructured materials, surfaces and interfaces</i> <b>Andrew Wheatley</b> <b>David Field</b> <b>Vincenzo Guidi</b> <b>Agata Kowalska</b>
10 <sup>50</sup> – 11 <sup>20</sup>	<b>Coffee break</b>

11 <sup>20</sup> – 13 <sup>10</sup>	<i>Morning session II:</i> <i>Nanostructured materials, surfaces and interfaces</i> <b>Beata Ziaja-Motyka</b> <b>Liv Hornekær</b> <b>Péter Herczku</b> <b>Sergei Piskunov</b>
13 <sup>10</sup> – 14 <sup>30</sup>	<b>Lunch</b>
14 <sup>30</sup> – 16 <sup>00</sup>	<i>Afternoon Session I:</i> <i>Reactivity and nanocatalysis</i> <b>Dmitry Momotenko</b> <b>Rodolphe Antoine</b> <b>Shiv Khanna</b>
16 <sup>00</sup> – 16 <sup>30</sup>	<b>Coffee break</b>
16 <sup>30</sup> – 18 <sup>30</sup>	<i>Afternoon Session II:</i> <i>Special session on the occasion of 80<sup>th</sup> birthday of Professor Jean-Patrick Connerade</i> <b>Nigel Mason &amp; Andrey Solov'yov</b> <b>Mike Mansfield</b> <b>Aslam Baig</b> <b>George Philip</b> <b>John Marangos</b> <b>Jean-Claude Lehmann &amp; Michel Broyer</b> <b>Chris Mayhew</b> <b>Stephen Hogan</b>

**Wednesday, April 26**

9 <sup>00</sup> – 10 <sup>30</sup>	<i>Morning session I:</i> <i>Propagation of particles through media</i> <b>Andrei Korol &amp; Andrey Solov'yov</b> <b>Werner Lauth</b> <b>Laura Bandiera</b>
10 <sup>30</sup> – 10 <sup>50</sup>	<b>Coffee break</b>
10 <sup>50</sup> – 12 <sup>30</sup>	<i>Morning session II:</i> <i>Design and practical realization of novel gamma-ray crystal-based light sources</i> <b>Davide De Salvador</b> <b>Konstantinos Kaleris</b> <b>Riccardo Negrello</b> <b>Thu Nhi Tran Caliste</b>
12 <sup>30</sup> – 12 <sup>40</sup>	<b>DySoN 2023 Closing</b>