Book of Abstracts

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PIER

Partnership of Universität Hamburg and DESY

PIER Graduate Week 2017

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Introduction

Welcome to the PIER Graduate Week 2017, an interdisciplinary workshop and lecture week for PhD students. Numerous national and international experts will offer a wide range of introductory and focus courses in the research fields Particle & Astroparticle Physics, Nanoscience, Photon Science, Infection & Structural Biology. Each course is a consecutive four-day series of lectures and/or workshops. The introductory courses are designed for doctoral candidates who would like to learn more about a related research field, while the focus courses are in-depth sessions for doctoral candidates in their own respective research area.

Speakers

Florian Bertram (DESY, Hamburg)
Celine Boehm (Durham University)
Karsten Büßer (DESY, Hamburg)
Henry Chapman (CFEL, DESY and Universität Hamburg)
Carsten Claussen (Fraunhofer ScreeningPort, Hamburg)
Ann-Christin Dippel (DESY, Hamburg)
Sonia Francoual (DESY, Hamburg)
Florian Grüner (Universität Hamburg)
Rolf Haug (Leibniz Universität Hannover)
Michael Hauschild (CERN, Genf)
Thomas Ihn (ETH Zurich)
Axel Knop-Gericke (Fritz Haber Institute, Berlin)
Martin Kroner (ETH Zurich)
Michael Kuhn (Universität Hamburg)
Jeroen Mesters (University of Lübeck)
Nacho Pascual (CIC nanoGUNE, San Sebastian)
Michael Rübhausen (CFEL)
Roland Wiesendanger (INCH and ZOQ, Universität Hamburg)
Carsten Wrenger (University of Sao Paulo)

Local organising committee

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Jochen Küpper (Photon Science)
Jenny List (Particle and Astroparticle Physics)
Markus Perbandt (Infection and Structural Biology)
Robin Santra (spokesperson PIER Helmholtz Graduate School)
Mirko Siemssen (administration PIER Helmholtz Graduate School)
Susanne Schuster (administration PIER Helmholtz Graduate School)
Matthias Kreuzeder (administration DESY)

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Programme

Monday, 9 October 2017

8:30 Registration
9:00 A1: Introductory course Particle and Astroparticle Physics (SR III)
A2: Introductory course Photon Science (SR II)
10:30 *Coffee break (CFEL foyer)*
11:00 B1: Introductory course Infection and Structural Biology (SR II)
B2: Introductory course Nanoscience (SR III)
B3: Introductory course Physics for Biologists (SR I)
12:30 *Lunch break*
14:00 C1: Focus course Particle and Astroparticle Physics (SR III)
C2: Focus course Photon Science (SR II)
C3: Competent at conferences (group A; SR V)
C4: Introduction to Scientific Computing in Python I (group A; building 3, SR III)
15:30 *Coffee break (CFEL foyer)*
16:00 D1: Focus course Infection and Structural Biology (SR II)
D2: Focus course Nanoscience (SR III)
D3: Competent at Conferences (group B; SR V)
D4: Introduction to Scientific Computing in Python I (group B; building 3, SR III)
17:30 *Coffee break (CFEL foyer)*
18:00 E1: Scientific colloquium and welcome reception (SR I- III)

Tuesday, 10 October 2017

9:00 A1: Introductory course Particle and Astroparticle Physics (SR III)
A2: Introductory course Photon Science (SR II)
10:30 *Coffee break (CFEL foyer)*
11:00 B1: Introductory course Infection and Structural Biology (SR II)
B2: Introductory course Nanoscience (SR III)
B3: Introductory course Physics for Biologists (SR I)
12:30 *Lunch break*
14:00 C1: Focus course Particle and Astroparticle Physics (SR II)
C2: Focus course Photon Science (SR III)
C3: Competent at conferences (group A; SR V)
C4: Introduction to Scientific Computing in Python I (group A; building 3, SR III)
15:30 *Coffee break (CFEL foyer)*
16:00 D1: Focus course Infection and Structural Biology (SR II)
D2: Focus course Nanoscience (SR III)
D3: Competent at Conferences (group B; SR V)
D4: Introduction to Scientific Computing in Python I (group B; building 3, SR III)
17:30 *Coffee break (CFEL foyer)*
18:00 E2: Business talk (SR I- III)

Wednesday, 11 October 2017

9:00 A1: Introductory course Particle and Astroparticle Physics (SR III)
A2: Introductory course Photon Science (SR II)
10:30 *Coffee break (CFEL foyer)*
11:00 B1: Introductory course Infection and Structural Biology (SR II)

B2: Introductory course Nanoscience (SR III)
B3: Introductory course Physics for Biologists (SR I)

12:30 *Lunch break*

14:00 C1: Focus course Particle and Astroparticle Physics (SR III)
C2: Focus course Photon Science (SR II)
C3: Competent at conferences (group A; SR V)
C4: Introduction to Scientific Computing in Python I (group A; building 3, SR III)

15:30 *Coffee break (CFEL foyer)*

16:00 D1: Focus course Infection and Structural Biology (SR II)
D2: Focus course Nanoscience (SR III)
D3: Competent at Conferences (group B; SR V)
D4: Introduction to Scientific Computing in Python I (group B; building 3, SR III)

17:30 *Coffee break (CFEL foyer)*

18:00 Poster Session (SR I- III)

19:00 E3: BBQ (CFEL atrium and café)

Thursday, 12 October 2017

9:00 A1: Introductory course Particle and Astroparticle Physics (SR III)
A2: Introductory course Photon Science (SR II)

10:30 *Coffee break (CFEL foyer)*

11:00 B1: Introductory course Infection and Structural Biology (SR II)
B2: Introductory course Nanoscience (SR III)
B3: Introductory course Physics for Biologists (SR I)

12:30 *Lunch break*

14:00 C1: Focus course Particle and Astroparticle Physics (SR III)
C2: Focus course Photon Science (SR II)
C3: Competent at conferences (group A; SR V)
C4: Introduction to Scientific Computing in Python I (group A; building 3, SR III)

15:30 *Coffee break (CFEL foyer)*

16:00 D1: Focus course Infection and Structural Biology (SR II)
D2: Focus course Nanoscience (SR III)
D3: Competent at Conferences /group B; SR V)
D4: Introduction to Scientific Computing in Python I (group B; building 3, SR III)

17:30 *Coffee break (CFEL foyer)*

Michael Hauschild (CERN), Introduction to Particle Physics (9-12 Oct)

The Standard Model of Particle Physics is one of the greatest successes in modern science. Its development started about 50 years ago and culminated in the discovery of the Higgs Boson at the CERN LHC collider in 2012. This was only possible due to a close interplay of theoretical physics and experimental physics together with advanced detector and accelerator technologies.

The lecture series will lead through the basic aspects of the standard model, covering also particle detectors and accelerators, with focus on the LHC collider and experiments. Recent LHC measurements and searches for physics beyond the Standard Model will be highlighted. Future world-wide projects and plans over the next decades will be presented.

Notes:

Sonia Francoual (DESY, Hamburg), Resonant X-ray magnetic scattering (9 Oct)

The development of modern synchrotron radiation sources providing polarized X-rays of tune-able wavelengths and high flux has strongly contributed to the establishment of magnetic X-ray scattering as a powerful method to probe magnetic structures in complement to neutron diffraction. Whereas non-resonant magnetic X-ray scattering allows it to separate the spin and orbital contributions to the total magnetization density and, in the high X-ray energy limit, to map the spin-only momentum distribution, resonant X-ray magnetic scattering is electron shell and element specific allowing it to determine the magnetic structure of different magnetic species and probe higher order multipoles order. In this lecture, I will introduce the basic concepts of magnetic X-ray scattering, describe the experimental set-up needed for state of the art experiments and illustrate the technique with recent scientific highlights.

Florian Bertram (DESY, Hamburg), X-ray diffraction on epitaxial thin films (10 Oct)

This lecture will focus on studies of epitaxial thin films. It will demonstrate how x-ray diffraction can be used to determine the structure of ultra-thin films and the interfaces between the films and the
substrate. In the first part theoretical considerations and typical instrumentation will be discussed. In the second part scientific examples will be presented to demonstrate how thin film x-ray diffraction is used in today's research.

Ann-Christin Dippel (DESY, Hamburg), Powder x-ray diffraction and pair distribution function analysis (11 Oct)

Many of the materials that we use in our everyday life are polycrystalline, amorphous, or nanocrystalline. Powder x-ray diffraction and pair distribution function analysis are very effective tools to study the structure of these kinds of materials. This lecture covers the basics of the methods as well as applications from (nano)materials science.

Vedran Vonk (DESY), X-ray diffraction from nano systems (12 Oct)

The atomic structure determination of nano-objects with dimensions in the sub-10 nm regime is a formidable task for today’s diffraction, imaging and scanning probe techniques. Such a detailed structural and compositional analysis is mandatory for a correlation with the nano-object’s functionality e.g. as heterogeneous catalysts, magnetic storage material or light emitting device. In conventional x-ray diffraction experiments on powder samples the structural analysis is hampered by a random nanoparticle orientation and often by background scattering from the supporting material. Here we will present different ensemble averaging in-situ synchrotron radiation based x-ray diffraction schemes delivering quantitative information on the nanoparticle size, shape and facet surface structures.

Notes:

Carsten Wrenger (University of Sao Paulo), Strategies to discover novel therapeutics to target human pathogens (9-12 Oct)

Diseases, caused by bacteria, viruses and parasitic protozoans belong to the principal challenges of human health. Globalization and increasing resistance of pathogens against drug intervention have led to a spread of infectious diseases. Therefore, this lecture - within the PIER week - intends to give first insights into the field of infectious diseases by focussing on human pathogens as well as their treatments. Besides an overview of the biology of selected parasites the current state of available molecular and biochemical tools to validate metabolic pathways as drug targets outside and inside of the pathogen will be illustrated. Subsequently the discovery of drugs/inhibitors against identified drug targets will be addressed by several approaches such as rational drug design by exploiting peculiarities of proteins which have been analysed at the structural level or by high throughput screening (HTS) studies against selected proteins of human pathogenic agents or at the cellular level.

Notes:

Thomas Ihn (ETH Zurich), Transport in Nanostructures at the level of single electrons (9-10 Oct)

Quantum dots give access to controlled single-electron and single-spin transport through artificial atoms and molecules and thereby provide insights into the fundamentals of the electrical current. We will introduce the relevant physics of charge carrier interactions, quantum confinement and tunneling, as well as thermodynamic aspects of transport. Along the way, we will touch material and fabrication aspects, and see how single electrons can be detected.

Martin Kroner (ETH Zurich), Quantum optics with quantum dots (11 Oct)

Single self-assembled semiconductor quantum dots (QDs) are the prime example of nano scale objects which allow us to test fundamental quantum mechanical concepts like photon anti-bunching and entanglement. These concepts play an important role in many applications of quantum mechanics for information technology.
In this lecture I will introduce the physics of QDs and how we can probe their optical properties and manipulate their quantum states by optical means. QDs are semiconductor structures and hence we can engineer their environment on the nano scale in order to control their electronic, spin, and optical properties. I will discuss how we can employ these techniques in order to generate entanglement between an electron, resident to the QD, and a photon that has been emitted by this same QD. Finally, I will conclude by discussing how this can be used to generate entanglement between two distant electrons resident in two distant QDs.

Martin Kroner (ETH Zurich), Nano-optics of two-dimensional semiconductors (12 Oct)

The optics of two-dimensional (2d) semiconductor structures is a rich field that allows us to investigate exotic quantum phenomena of matter and light. While most of the state of the art experiments of this sort are being performed in the "classical" III-V or II-VI semiconductor
heterostructures, I will start this lecture by introducing a new class of materials that has emerged recently, namely monolayers of transition-metal dichalcogenides (TMDs) that can be embedded in van-der-Waals heterostructures. I will discuss some of their fascinating optical properties and how they allow new insight into some old problems of 2d semiconductor optics. If time permits, I will end this lecture by giving a glimpse into the rich field of cavity quantum electrodynamics with both
TMD and GaAs heterostructures.

Notes:

Karsten Büßer (DESY, Hamburg), The quest fort the smallest and largest structures in the universe (9 Oct)

What are the smallest building blocks in nature and how do they react under the elementary forces? How do the rules of the microcosm influence the macrocosm on its largest scales in the universe? These fundamental questions are the heart of the particle physics research worldwide.

DESY is a leading player in the worldwide experimental and theoretical research in particle and astroparticle physics. DESY groups participate in experiments at the largest particle collider, the LHC at CERN, at the Belle-II detector in Japan and in the on-site non-collider experiment ALPS-II. DESY groups in Zeuthen have leading roles in experiments that exploit particles from the cosmos and open paths to understand the mechanisms of cosmic particle accelerators.

After decades of research, still many open questions about the fundamental structure of our universe remain. What are the unknown constituents of the universe, the Dark Matter and the Dark Energy? How do they influence the history and the fate of the universe? What is the role the Higgs particle - that has been discovered at the LHC in 2012 - in this game?

DESY pushes R&D for future accelerators and experiments that will help to answer the big open questions about the fundamental structures of our world.

Henry Chapman (CFEL, DESY and Universität Hamburg) Imaging of Macromolecular Structures (10 Oct)

I will explain concepts in imaging and structure determination and use them to discuss some familiar methods such as microscopy, tomography, crystallography, and holography. Such methods can be used with light (photons), electrons, or other particles. I will give emphasis on ways to achieve high enough resolution to visualise molecules, and will describe differences between techniques based on properties of the radiation and its interaction with matter.

Michael Rübhausen (CFEL), Physics of transition metal complexes (11 Oct)

The Chemistry and Physics of transition metal complexes is critical for many biological functions such as skin pigmentation, immunological defense mechanisms, or oxygen transport.
By using a combination of modern optical and X-ray techniques I will outline how the biochemical and biophysical mechanisms behind these processes can be revealed. Beyond that mankind has learned to adapt mechanisms developed by nature to make use of them.
Finally I will briefly sketch how the future developments in modern X-Ray science will benefit the research and understanding of transition metal chemistry and physics in these systems.

Florian Grüner (Universität Hamburg), From laser-driven X-ray sources to medical imaging (12 Oct)

Medical imaging is a very active field of interdisciplinary research, with the aim of developing new schemes with unprecedented sensitivity, for instance for early tumor diagnostics. One of the candidates for such new imaging modalities is X-ray fluorescence imaging (XFI), using excited X-ray emission from functionalized gold nanoclusters.

In this presentation you will learn about the basics of XFI as well as the physics of laser-driven X-ray sources, which can deliver X-ray beams with high brilliance, the key to such new imaging modalities.

Notes:

Celine Boehm (Durham University), The invisible Universe: What do we know about dark matter? (9-12 Oct)

About 95 % of the content of the Universe appears to be of mysterious nature. While this modern realisation challenges our understanding of the fundamental laws of Physics, it also promises great discoveries ahead, and a possible shift in paradigm comparable to the Copernican revolution. In this talk, I'll focus on dark matter and the knowledge we have acquired so far.

Notes:

Axel Knop-Gericke (Fritz Haber Institute, Berlin), Ambient pressure Photoelectron Spectroscopy of catalytically active interphases (11-12 Oct)

In my lectures photoelectron spectroscopy will be introduced as a method which enables the investigation of the electronic structure of catalytically active solid-gas phase interphases. The application of this technique allows the study of correlations between the electronic structure of catalysts surfaces and the catalytic performance. These correlations are required to understand the reaction mechanism of the catalytic reaction. A few examples of studied heterogeneous catalytic reactions like the methanol oxidation over copper will be discussed.

Since the energy supply of the future is rested upon renewable energies, the storage of energy is in the focus of energy research. One approach bases upon the synthesis of chemical compounds like methanol or ammonia using hydrogen, which was obtained by electrochemical water splitting. The processes which occur at the electrode surfaces during water splitting are not well understood. I will demonstrate that ambient pressure X-ray photoelectron spectroscopy can be applied to investigate electrochemically active solid-liquid interfaces as well. The oxygen evolution reaction will be discussed in detail.

Notes:

Jeroen Mesters (University of Lübeck), Introductory course Infection and Structural Biology (9-12 Oct)

Central concepts in (bio)crystallography:
1. Solubility phase diagram and crystallogenesis
2. Bragg's law and the Ewald sphere construction
3. Patterson function and method
4. Electron density maps

Obtaining 3D structural information, i.e. near atomic, medium to high resolution or even atomic resolution, is a key step in the analysis of structure-function relationships of biological macromolecules. The most important method for obtaining this information is bio-crystallography (more than 89% of all structures listed in the RSCB Protein Data Bank). Hence, we will address a few central concepts in biocrystallography that must be tackled during the mission from protein stock solutions to interpretable electron density maps.

Notes:

Rolf Haug (Leibniz Universität Hannover), Single-Electron Tunneling through Quantum Dots: Shot Noise and Counting Statistics (9-10 Oct)

Electronic transport through quantum dots, i.e. quasi zero-dimensional systems in semiconductors, is governed by single-electron tunneling and Coulomb interactions. Due to the discrete nature of the tunneling events shot noise appears in the measured current. Additionally detectors even allow to monitor the tunneling of individual electrons and the quantum statistics of the tunneling events can be obtained [1,2]. In applying feedback and pumping schemes counting statistics can be manipulated and shot noise can be suppressed [3,4].

[1] C. Flindt, C. Fricke, F. Hohls, T. Novotný, K. Netočný, T. Brandes, R.J. Haug, Proc. Nat. Acad. Sci. 106, 10116 (2009).
[2] N. Ubbelohde, C. Fricke, C. Flindt, F. Hohls, R.J. Haug; Nature Comm. 3, 612 (2012)
[3] N. Ubbelohde, F. Hohls, V. Kashcheyevs, T. Wagner, L. Fricke, B. Kästner, K. Pierz, H.W. Schumacher, R.J. Haug; Nature Nanotech. 10, 46 (2015)
[4] T. Wagner, P. Strasberg, J.C. Bayer, E.P. Rugeramigabo, T. Brandes, R.J. Haug; Nature Nanotech. 12, 218 (2017)

José Ignacio Pascual (CIC nanoGUNE, San Sebastian), Exciting Electrons, Spins, and Vibrations in atoms and molecules, one at a time (11-12 Oct)

The development of scanning tunneling spectroscopy at low temperatures during the last decades facilitated the access to a large variety of fundamental phenomena in individual atoms and molecules, magnetism, optics, chemistry,…. many of which were unexpected years ago. Tunneling electrons probe electronic density of states in an elastic and coherent manner. But they also are highly controllable a source of incoherent excitations, exchanging energy, and angular momenta with the states of an atom/molecule/surface.
In the course of two lectures I will advance though some (not all) of the most recent research fields accessed by tunneling spectroscopy, and, in particular:

- The electronic structure of surfaces: quasiparticle scattering revealing band structure
- Molecular states and their excitations: Vibrations, photons, electrons, and spins…all in an atom
- Excitations on a superconducting surface: quasiparticle density of states revealing spin and cooper-pair excitations

Notes:

Roland Wiesendanger (Interdisciplinary Naoscience Center Hamburg and Center for Optical Quantum Technologies, Universität Hamburg), From Skyrmions to Majoranas: Nanoscience Inspired by Particle Physics Theory (9 Oct)

Modern solid state physics has become greatly inspired by particle physics theories in recent years. The reason is that quasiparticles are a very useful concept for understanding complex phenomena in many-body physics. Recent outstanding examples are Skyrmions as topological defects in vector fields characterized by a topological charge, or the Majoranas, i.e. particles being their own antiparticles and therefore chargeless. The lecture will focus in the first part on the discovery of single chiral magnetic skyrmions in ultrathin metallic films, made at the University of Hamburg in 2013, and their potential applications in future ultrahigh-density magnetic memory and logic devices. In the second part, the lecture will focus on the exciting search for Majoranas in atomic-scale model systems with great potential for future quantum information and communication technologies.

Carsten Claussen (Fraunhofer ScreeningPort), Career paths in science and beyond (10 Oct)

Can you plan a career? How to become happy? Can you calculate your business success? Based on his own career, Carsten Claussen will talk about the demands of big and small industry, as well as of research in and outside universities. He will discuss and sharpen "Good Advice" such as generating chances, networking, implementing own visions, diligence and endurance, the ratio of fun & frustration and the salary's worth using positive and negative examples.

Notes:

Jan-Hendrik Arling, Characterization and Design Optimization of Petals as Local Support Structures for the ATLAS ITk Strip Detector (Particle & Astroparticle Physics)

The ATLAS Phase-II Inner Tracker (ITk) Strip Detector is an upgrade of the current ATLAS tracking detector for the challenges of the high-luminosity LHC, planned for 2026. The ITk detector of ATLAS is a full-silicon pixel and strip tracking detector with highest precision and withstanding large radiation doses.

The forward regions (the "end-caps") of the silicon strip tracker will consist of six disks populated with wedge-shaped silicon micro-strip sensors, divided in "module" units containing the readout, power and control electronics.

The modules are directly glued on likewise wedge-shaped local support structures called petal cores, consisting of carbon fiber-based sandwich structures with embedded titanium cooling pipes as well as data and power buses.

The combination of a petal core plus 18 sensor modules of six different shapes glued on it is called petal. Each end-cap disk is constituted of 32 petals. The petal core structure provides mechanical stability for the glued on sensor modules while minimizing the amount of material. Evaporative CO_2 cooling is used to allow for cooling of the sensors as well as the readout electronics.

During the optimization stage of the petal design, a number of petal cores, as well as a thermo-mechanical petal fully loaded with dummy silicon modules, were built. Extensive tests of these prototypes are being performed, with the aim to address their mechanical stability (e.g. bending and vibration), thermo-mechanical characteristics (e.g. infrared imaging) and material properties (e.g. radiation length measurements).

A variety of such results, as well as the comparison with FEA simulation results, will be presented on this poster.

Parisa Bayat, Plasmonics and Nanofluidics for DNA-Single Molecule Detection (Nanoscience)

Parisa Bayat, Irene Fernandez-Cuesta, Franziska Esmek, and Robert H. Blick

Plasmonic antenna nano-focus the light beyond diffraction. These hot spots are ultra-sensitive, what can be exploited for single molecule (bio) sensing. But there is a major challenge: placing the target element at the sensitive area. Here, we have integrated a sub-100nm nanochannel crossing the antenna gap, what allows the in-line detection of single molecules of DNA in real-time as they pass through the light "hot-spot". In this configuration, the molecules are detected as peaks in the fluorescent signal in time scans. This allows real time read-out of the molecules with no limitation in the length and without an expensive camera.

For total liquid control, the nanochannel is connected to a complete fluidic system. This represents a new type of super-sensitive (bio) sensor, with singlemolecule real time detection capabilities.

We have developed a wafer-scale fabrication process, based on nanoimprint lithography [1], to make the complete fluidic devices in one single step, only 120 seconds.

Discrete DNA molecules have been detected and counted by in-line detection in real time. Different types of viral DNA molecules (λ-Bacteriophage and Kaposi's sarcoma herpesvirus) were stained with intercalating dyes and stretched in the nanochannels.

[1] I. Fernandez-Cuesta et al., J. Vac. Sci. Technol. B29, 06F801 (2011)

Intissar Chahbani, Nanobody based immunoassay for rapid and sensitive detection of Clostridium difficile Toxins (Infection & Structural Biology)

Intissar Chahbani[1,2], Maria Pilar Mejias3, Lucas Schumacher[1], Imed Salhi[2], Klaus Aktories[4], Marina Palermo[3], Hans-Willi Mittrücker[1], Touhami Korchani[2] and Friedrich Koch-Nolte[1]

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Clostridium diffcile is the major cause of antibiotic associated diarrhea and pseudomembranous colitis in Europe and North America. The incidence of the pathogen has increased dramatically worldwide during the last decade leading to a high morbidity and mortality rates. This outbreak has been associated with the emergence of hyper virulent strains (BI/NAP1/027) that produce additionally to ToxA and ToxB, which have a glycosylating activity, a third binary Toxin called CDT an actin-specific ADP-ribosyltransferase which consists of two sub units CDTa an enzymatic component and CDTb as a binding component.

The incidence of Treatment failure with traditional antibiotics, low sensitivity of diagnostic immunoassays and high recurrence of Clostridium diffcile infection make the Nanobodies a promising tool for diagnostics and treatment owing to their reproducibility, stability, and cost-effective production.

The purpose of this study was to develop a Nanobody-based strategy for rapid, and sensitive detection of C. diff Toxins in biological samples since variance between diagnostic tests is an ongoing barrier to clinical decision making.

Nanobodies specific to ToxB and CDTb were selected from an immune VHH library obtained from immunized dromedaries by phage display technology. The selected VHHs recognizing non overlapping epitope were selected for setting the capture /detector pairs of a sandwich ELISA. The detector Nanobodies were conjugated with Biotin molecules which bind with high affinity to the strepdavidin.

We have successfully constructed a high quality phage display VHH library and isolated nine and five (VHHs) distinct families against CDTb b and ToxB respectively after biopanning. All selected VHHs have been shown to bind specifically to their target with high affinity.

The established ELISA exhibited a detection limit of 0.3ng/ml and 0.1ng/ml for CDTb and ToxB respectively and was able to detect specifically the Toxins in mice stool samples infected with C.diff spores.

The proposed immunoassay offers great promises in providing a rapid, inexpensive, sensitive and specific detection of C.diff toxins in clinical settings.

Deniza Chekrygina, Real time morphological investigation of bimetallic nanoparticles during dual-sputtering of Au/Ag. (Photon Science)

D. Chekrygina[1], M. Schwartzkopf[2], A. Rothkirch[2], P. Pandit[2], I. Baev[1], F. Kielgast[1], Jan Rubeck[2], S.V. Roth[2,3], W. Wurth[1,2], M. Martins[1]

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Polymetallic nanoparticles and thin films containing Au in combination with other metals tend to be promising candidates for production of novel materials. By ratio variation of the metals in the system one can significantly affect the physical and the chemical properties, which opens their possible application as e.g. catalysts, sensors or photonic devices.

In this work we focused on the simultaneous deposition of 10 nm of Au and Ag from dual sources and investigated changes in real time in morphology and optical properties. This was achieved by combining in situ Grazing Incidence Small Angle X-ray Scattering (GISAXS) technique with UV/Vis reflectance spectroscopy at the P03 beamline, PETRA III, at DESY in Hamburg.

We will present a comparison of the physical and structural properties of a simultaneously sputtered Au/Ag alloy with an alternate deposition and a pure metal deposition. Furthermore the effect of temperature during the deposition will be discussed.

Ángel Ferran Pousa, External Injection Into a Laser-Driven Plasma Accelerator With Sub-Femtosecond Timing Jitter (Accelerator Physics)

The use of external injection in plasma acceleration is attractive due to the high control over the electron beam parameters, which can be tailored to meet the plasma requirements and therefore preserve its quality during acceleration.

However, using this technique requires an extremely fine synchronization between the driver and witness beams. In this poster, we present a new scheme for external injection in a laser-driven plasma accelerator that would allow, for the first time, sub-femtosecond timing jitter between laser pulse and electron beam.

Sravya Mounika Kantamneni, Recent developments in ARP/wARP (Infection & Structural Biology)

Sravya Kantamneni, Grzegorz Chojnowski, Joana Pereira, Daria Beshnova, Philipp Heuser, Umut Oezugurel, Victor Lamzin

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The ARP/wARP software project [1,2] combines automated model building and refinement for macromolecular crystal structure determination. The project itself is the result of more than two decades of extensive research and development in the areas of macromolecular X-ray crystallography, informatics, data mining, and statistical pattern recognition. ARP/wARP collects vast amount of computationally efficient methods and provides easy-to-use pipelines for building models of proteins, nucleotides, small molecules, as well as their complexes.

Here we present recent innovations of ARP/wARP that improve performance at low resolution and enable interpretation of cryo-electron microscopy (cryo-EM) maps. The main-chain tracing tools for both proteins and nucleic acids now incorporate new algorithms that yield more reliable models with better local geometry. The protein side-chain docking module has been completely redesigned that resulted in improved performance, at low resolution in particular. ARP/wARP provides also a new, fully automated tool for building atomic models of proteins and nucleic acids into high-resolution cryo-EM maps. Finally, we redesigned our web-server that now provides all the ARP/wARP functionalities.

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[2] Langer, G.G. et. al. (2013), Acta Cryst. D69, 635-641.

Thomas Kotzott, Insight into a solid with atomic resolution: scattering at single impurities (Nanoscience)

Thomas Kotzott and Martin Wenderoth

The scanning tunneling microscope (STM) is mostly known as tool for surface science that provides structural and electronic information on the atomic scale mapping the local density of states. Beyond that the STM can be used with different techniques in a variety of fields like local surface transport properties and local dynamics on short time scales.

However, the STM occasionally can also give an insight into the solid and then reveals a powerful combination of atomic lateral resolution and probing bulk properties. The electron focusing effect [1] lets electrons propagate long distances of multiple nanometers through a metal crystal without being effectively damped. This is possible along paths of specific direction which are determined by the band structure of the host material, e.g. the Fermi surface. Mapping the interference pattern of electrons scattered at an impurity within the bulk and then travelled coherently to the surface yields access to the nature of the scattering process on the atomic level. Hence, a look at the surface of the sample reveals information about single atoms within the sample.

Here, we investigate the scattering of bulk electrons at single, non-magnetic impurities. Dilute alloys of germanium in copper are prepared in-situ under UHV conditions. Cu and the impurity material Ge are simultaneously evaporated from electron beam evaporators onto a single crystal Cu(100) surface which is previously cleaned by cycles of argon bombardment and annealing. Scanning tunneling microscopy and spectroscopy was performed using a home-built low-temperature STM operating at 6 K. Topography data reveals ring-like features in the local density of states (LDOS) with electronic contrasts down to few picometers in height. Spectroscopy accesses the differential conductance with energy resolution and therefore resolves the scattering of different bulk states at the impurity.

Miriam Künzel, CP violation measurement at the Belle II experiment (Particle & Astroparticle Physics)

CP violation is one of the key aspects of physics beyond the Standard Model. This symmetry violation can be measured at colliders working as B meson factories, for instance the Belle II experiment, which is currently being built at the KEKB collider in Japan.

This poster gives a short overview over some of the theoretical aspects of CP violation, as well as the Belle II detector components and the combinatorial Kalman filter implemented by me as an example for a Belle II tracking algorithm.

Pirmin Lakner, Planar and porous polypyrrole/silicon hybrid material systems (Photon Science)

Pirmin Lakner[1], Manuel Brinker[2], Andreas Stierle[1], Patrick Huber[2], Thomas Keller[1]

The investigation of interfaces in two-dimensional planar systems plays an elementary role in the investigation of porous hybrid materials, since it allows effects in more complex geometries to be attributed to their underlying causes.

For the analysis of polypyrrole/silicon hybrid material systems, an electrochemical cell has been developed that enables the in-situ and nanometer-accurate investigation of the electropolymerization of pyrrole on planar silicon crystals using X-ray reflectometry. At the same time, electron density profiles and characteristic potential curves are recorded and layer heterogeneity is measured using SEM and AFM.

The electrochemical cell enables the investigation of the voltage-induced swelling behaviour of polypyrrole, which opens up possible applications of porous polypyrrole/silicon hybrid material systems as actuators or sensors and optimizes them with regard to mechanical and electrical properties.

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[2] TU Hamburg-Harburg, Institut für Werkstoffphysik und Werkstofftechnologie

Jhilik Majumdar, Spectral modulation of Galactic Gamma-ray sources due to photon-ALPs mixing in Galactic magnetic field (Particle & Astroparticle Physics)

Jhilik Majumdar, Francesca Calore, Dieter Horns

Axion like particles (ALPs) are fundamental pseudo scalar particles with properties similar to Axions that have been invoked to solve the strong CP problem in Quantum Chromodynamics. ALPs can oscillate into photons and vice versa in the presence of an external magnetic field. This oscillation of Photon and ALPs could have important implications for astronomical observations, i.e. a characteristic energy dependent attenuation in Gamma ray spectra for astrophysical sources.

Here we have revisited the opportunity to search Photon-ALPs coupling in the disappearance channel. We use nine years of Fermi Pass 8 data of a selection of Galactic Gamma-ray source candidates and study the modulation in the spectra in accordance with Photon-ALPs mixing and estimate best fit values of the parameters i.e. Photon-ALPs coupling constant ($g_{\alpha\gamma}$) and ALPs mass (ma). For the magnetic field we assume large scale galactic magnetic field models based on Faraday rotation measurements.

Nils Roth, Numerical simulations for characterizing and optimizing an aerodynamic lens (Photon Science)

Nils Roth[1], Salah Awel[1,3], Daniel Horke[1,3] and Jochen Küpper[1,2,3]

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With coherent diffractive imaging at free-electron lasers it is possible to reconstruct the three-dimensional molecule structures of isolated particles at atomic resolution. However, this requires reproducible samples [1].

Currently one of the major limiting factors is the inefficient delivery of particles and the correspondingly low number of strong diffraction patterns, collected during typical beam times. We build a numerical simulation infrastructure capable of calculating the flow of gas and the trajectories of particles through an entire aerosol injector, aiming to increase the fundamental understanding and to enable optimization of injection geometries and parameters.

The simulation results are compared to literature studies and also validated against experimental data taken in an aerosol beam characterization setup [2]. The simulation yields a detailed understanding of the radial particle distribution and highlights weaknesses of current aerosol injectors. With the aid of these simulations we develop new experimental implementations to overcome current limitations and increase particle densities available for diffractive imaging experiments.

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[2] S. Awel, R. A. Kirian, N. Eckerskorn, M. Wiedorn, D. A. Horke, A. V. Rode, J. Küpper, H. N. Chapman, Opt. Exp. 24, 6507-6521 (2016)

Mia Rudolph, Experimental phasing for intracellular protein crystallography (Infection & Structural Biology)

J. Mia Rudolph, Winnie Riekehr, Christopher Klapproth, Robert Schönherr, Lars Redecke

Protein crystallization in living cells -in vivo crystallization- holds the possibility to grow a huge number of micron-sized crystals. Comparable properties and a high order of the proteins in the crystal lattice together with the short time needed for crystal growth results in an enormous potential for structural biology. We are establishing serial X-ray crystallography as a pipeline with recombinant proteins that form microcrystals in living insect cells: InCellCryst, from cloning over detection to mounting techniques at advanced X-ray sources, serial data collection (both at synchrotron sources or FELs) and structure elucidation.

A current bottleneck is the varying proportion of cells carrying protein crystals, depending on a multitude of interconnected and largely unknown factors. Moreover, Molecular Replacement is required to solve the phase problem so far, resulting in the elucidation of three high-resolution structures from different proteins.

A major aim of this project is to collect diffraction data of protein crystals within the living cell that can be experimentally phased at the same time. The most important issue is the labelling of proteins inside living cells. We are developing two approaches: 1) SeMet incorporation. Crystal production followed our InCellCryst pipeline in Met-deficient medium with SeMet supplements. X-ray fluorescence emission spectra of isolated crystals already revealed incorporation of SeMet into intracellular protein crystals. 2) Lanthanide labelling. Terbium bound to a cell-penetrating-peptide is transferred to the target protein via a lanthanide-binding-tag. So far, neither SeMet incorporation nor tag-attachment have inhibited crystal formation. Serial diffraction data collection and experimental phasing following established protocols are in progress.

Experimental phasing of serial diffraction data of intracellular protein crystals will broaden the application spectrum of our pipeline to proteins without known homologue structures, usually difficult to crystallize using conventional methods.

Rustam Rysov, Probing ultra-fast dynamics with the hard X-ray delay line (Photon Science)

Probing condensed matter on the timescales from femtoseconds to picoseconds is currently one of the key topics for future investigations of existing FEL sources. Modern X-ray sources are able to deliver highly intense femtosecond photon pulses with timegap of 769ps in between. It allows performing time resolved experiments. But in fact, for many applications which concerned with the electronic dynamics processes, the mentioned time gap between the pulses is still too long. One way to overcome this limitation is usage of split and delay unit. Such device can provide a tunable delay time between the photon pulses at the sample position independently of the time structure of the source.

Achieving pico- and femtosecond delays between two pulses with preserving FEL beam spatial parameters, shape and coherence can effectively use the advantage of FEL brilliance. It has scientific cases in many research directions such as molecular dynamics, femtosecond Fourier holography, Time-resolved magnetic scattering and ultrafast demagnetization studies. Additionally, for double pulse X-ray photon correlation spectroscopy it is highly necessary to have two pulses, delayed between each other propagating along the same path with a precisely measured delay time. This gives an opportunity to make contrast-based studies of dynamics in a various sample systems.

The split and delay system is designed to work in hard X-ray energy range from 8 to 15 keV to achieve delays covering the range between two successive FEL pulses and to go below the zero delay point (when two pulses arrive to the sample at the same time) in total from -10 to 605 picoseconds. This attractive delay time range give an opportunity to perform experiments, which require a temporal separation in the femtosecond and near-picosecond delay time ranges enabling the possibility of holding a various types of experiments depending on the timescale. Although, the delay unit itself have compact design of 60x60 centimeters with total weight less than 100kg. Such dimensions are compatible with the beamlines hardware and can be easily installed and operated independently.

The setup is using crystal optical elements in Bragg geometry to split an X-ray pulse into two fully adjustable fractions with defined geometry. It consists from beam splitter, Bragg crystal and channel-cut in order to achieve a different delay times and output beams directions. X-ray cameras and Avalanche PhotoDiodes (APD) are used for diagnostics and fine tuning.

Split pulse techniques enable the experimental investigation of structural dynamics with X-ray techniques by directly following the time evolution of the electron density during the course of a photo-induced biological, chemical or physical transformation.

Hendrik Schlicke, Electrostatically Actuated Membranes of Cross-Linked Gold Nanoparticles: Novel Concepts for Electromechanical Gas Sensors (Nanoscience)

H. Schlicke, S. C. Bittinger, M. Behrens, M. Yesilmen, H. Hartmann, C. J. Schröter, G. T. Dahl, T. Vossmeyer

Organically cross-linked gold nanoparticles (GNPs) represent novel composite materials with tunable optical and electronic properties. Further, they show the ability to sorb analyte molecules. Their perturbation-sensitive tunneling-based charge transport mechanism renders the materials interesting for sensing applications. While many studies focus on the fabrication and characterization of substratesupported thin films consisting of these materials, the investigation of freestanding membranes with nanoscale thickness was reported more recently. Coupling the mechanical properties of such GNP composite membranes to their electronic properties and sorption capabilities enables the fabrication of novel hybrid micro- and nanoelectromechanical systems (MEMS/NEMS) for sensing applications.

Herein, we present novel concepts for micro-/nanoelectromechanical chemical gas sensing, employing GNP membrane actuators[1] and resonators[2]. By applying DC or AC voltages, electrostatic forces were utilized to quasi-statically deflect (quasi-static method) freestanding GNP membranes, or to excite their vibrational resonances (dynamic method). We show that the observed voltage-deflection relations (quasi-static method) or resonance frequencies (dynamic method) are significantly influenced by sorption-induced changes of the membranes' mechanical properties and can hence be utilized as sensing signals for the detection of different vapors under reduced pressure (dynamic method) or ambient conditions (quasi-static method).[3,4] The new transduction principles can further be combined with chemiresistive sensing using GNP composites[5] and provide input for multivariable sensing applications.

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[3] H. Schlicke, M. Behrens, C. J. Schröter, G. T. Dahl, H. Hartmann, T. Vossmeyer, ACS Sens. 2017, 2, 540-546.
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Sarah Schroeder, Double bunch production for a beam driven plasma wakefield accelerator at FLASHForward (Accelerators)

S. Schröder[1,2], A. Aschikhin[1], J. Dale[1], R. D'Arcy[1], V. Libov[1,2], A. Martinez de la Ossa[2], T. Mehrling[1,2], L. Scharper[1], B. Schmidt[1], S. Wesch[1], J. Zemella[1] and J. Osterhoff[1]

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An ever increasing demand for high-energy accelerator systems is being witnessed in both fundamental research as well as industry. However, due to their large scale, conventional accelerators are not only unsuitable for practical applications but also costly. The limiting factors for compact conventional radio-frequency (RF-) accelerators are dissipation and electrical as well as material breakdown at high amplitudes of the accelerating electromagnetic field.

Such accelerating fields also occur as an intense laser beam or a high-current relativistic particle beam is focused onto a capillary filled with plasma. The amplitude of these plasma wakefields (GV/m) exceed the todays RF-fields by several orders of magnitude making plasma based acceleration a promising development towards smaller and accordingly cheaper accelerator facilities. FLASHForward (Future oriented wakefield acceleration research and development at FLASH) is a project dedicated to beam-driven plasma acceleration and is situated beside the FLASHII beamline at DESY. Primary objectives are the preservation of beam quality after plasma based acceleration of ultra-relativistic electrons, the creation of high-brightness electron beams and the demonstration of FEL (Free Electron Laser) operation based on plasma acceleration.

One particular acceleration method studied at FLASHForward utilises a driving ultra-relativistic electron bunch from the FLASH accelerator for plasma wakefield creation. A trailing electron bunch injected into the formed wakefield is then accelerated. The characteristics of the driving and trailing bunches such as charge distribution and emittance have a significant influence on the properties of the final plasma accelerated electron bunch.

The production of the consecutive driving and trailing bunch in the FLASHForward beamline and resulting simulations of the acceleration process are discussed in the poster.

Joana Valerio, SAXS and WAXS studies on liquid microjets (Photon Science)

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Liquid jets are used in synchrotron and XFEL experiments allowing studies of structure and dynamics of soft condensed matter. We developed a liquid jet setup for x-ray scattering experiments on complex fluids that supports small and wide angle x-ray scattering geometries (SAXS and WAXS) [1].

The jet is formed by a gas dynamic virtual nozzle (GDVN) [2] producing diameters ranging between 1 µm and 20 µm at a jet length of several hundred µm. The homogeneous and very thin liquid jets offer numerous advantages compared to conventional sample injection environments [1]. For instance, they allow measurements in a steady jet regime that breaks into a train of droplets cooling rapidly in vacuum and thus allowing studies on supercooled liquids [3].

In this presentation we will focus on two different studies using our liquids jet setup: 1) Flow-induced alignment of spindle-shaped particles probed by WAXS. 2) Influence from refraction of X-rays from µm-sized jets and droplets on the SAXS patterns; see Figure 1. Such anisotropic patterns arise due to the cylindrical (jet) and spherical (droplets) geometries [4].

Results will be compared with data taken with different injection devices and the possibility of performing rheology studies at high shear rates using liquid jets [5] will be discussed.

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Irene Zoi, Beam Test Results of Thin n-in-p 3D and Planar Pixel Sensors for the High Luminosity LHC Tracker Upgrade at CMS (Particle & Astroparticle Physics)

The poster will describe the development of new 3D and planar silicon pixel detectors designed for the CMS (Compact Muon Solenoid) Phase-2 Upgrade at HL-LHC (High Luminosity LHC). The project is funded by INFN, and produced in collaboration with the FBK foundry.

In the HL-LHC data taking period the instantaneous luminosity will be approximately 5 times larger than the original LHC design luminosity. This will, on one hand, increase the discovery potential and measurement precision at the experiments but on the other hand will significantly increase the radiation dose and the number of concurrent collisions per bunch crossing that will have to be sustained by the detectors.

In order to cope with these future conditions, upgrades to the detectors are required.

This is particularly necessary for the inner pixel tracker that is the closest to the proton-proton interaction point.

In this poster thin (100μm and 130μm thick) n-in-p type sensors, assembled into hybrid single chip modules bump bonded to the PSI46dig readout chip, currently used in the CMS experiment, will be presented.

Results from beam tests performed at Fermilab Test Beam Facility obtained with planar sensors before and after proton irradiation up to 3x1015 neq/cm2 will be described. It will also report on the first results reached with 3D pixel sensors 130μm thick with columnar electrodes for different pixel cell prototypes. The 3D prototypes have different unit pixel cell size, ranging form the standard 100μm x 150μm as used in the present CMS Pixel Tracker, down to 50μm x 50μm and 25μm x 100μm which are the most favored dimensions to cope with the harsh environment foreseen in the pixel tracker for the High Luminosity era.

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