PIER Graduate Week 2019

Interdisciplinary lecture and workshop week for PhD students

National and international experts offer a wide range of introductory lectures and in-depth focus courses in the research fields:

/ Particle & Astroparticle Physics

/ Nanoscience

/ Photon Science

/ Infection & Structural Biology

23 – 26 SEPT '19

BOOK OF ABSTRACTS

Programme & registration:
graduateschool.pier-hamburg.de/gradweek2019

Registration open until:
1 September 2019

/ Zlatan Akšamija
University of Massachusetts Amherst

/ Sebastian Busch
GEMS at Heinz-Maier-Leibniz Zentrum, Garching & Helmholtz-Zentrum Geesthacht

/ Diana Deterra
Freiheitsgrade Hamburg

/ Maria Garcia Alai
European Molecular Biology Laboratory & Center for Structural Systems Biology, Hamburg

/ Rebeca Gonzalez Suarez
Uppsala University

/ Eleftherios Goulielmakis
University of Rostock

/ Mark Hartney
SLAC National Accelerator Laboratory, Stanford University / Breakthrough Energy Ventures

/ Andreas K. Hüttel
University of Regensburg

/ Elena Kaufman
Creative Communications EK

/ Franz Kärtner
DESY and Universität Hamburg

/ Boris Krichel
Heinrich Pette Institute, Leibniz Institute for Experimental Virology, Hamburg

/ Vadim Kotov Universitätsklinikum Hamburg-Eppendorf & Center for Structural Systems Biology, Hamburg

/ Jan Kosinski
EMBL Hamburg, Centre for Structural Systems Biology Hamburg & Structural and Computational Biology Unit EMBL, Heidelberg

/ Francesco Pietro Massel
University of South-Eastern Norway

/ Gudrid Moortgat-Pick
Universität Hamburg

/ Geoffrey Mullier
Lund University

/ Eike Schulz
Max Planck Institute for the Structure and Dynamics of Matter, Hamburg

/ Christine Silberhorn
Paderborn University

/ Charlotte Uetrecht
Heinrich Pette Institute, Leibniz Institute for Experimental Virology, Hamburg & European XFEL, Schenefeld

PIER
Partnership of Universität Hamburg and DESY

Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

DESY.

PIER Helmholtz Graduate School
A Graduate Education Program of Universität Hamburg in Cooperation with DESY

Introduction

Welcome to the PIER Graduate Week 2019, 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

Zlatan Aksamija (University of Massachusetts Amherst, NanoEnergy & Thermophysics (NET) Lab)

Sebastian Busch (German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Garching & Helmholtz-Zentrum Geesthacht GmbH)

Maria Garcia Alai (European Molecular Biology Laboratory & Center for Structural Systems Biology, Hamburg)

Rebeca Gonzalez Suarez (Uppsala University)

Eleftherios Goulielmakis (University of Rostock)

Mark Hartney (SLAC National Accelerator Laboratory, Stanford)

Andreas K. Hüttel (University of Regensburg)

Franz Kärtner (DESY & Universität Hamburg)

Boris Krichel (Heinrich Pette Institute, Leibniz Institute for Experimental Virology)

Vadim Kotov (Universitätsklinikum Hamburg-Eppendorf & Center for Structural Systems Biology, Hamburg)

Jan Kosinski (EMBL Hamburg, Centre for Structural Systems Biology Hamburg &Structural and Computational Biology Unit EMBL, Heidelberg)

Francesco P. Massel (University of South-Eastern Norway, Dept. of Science and Industry systems)

Gudrid Moortgat-Pick (Universität Hamburg)

Geoffrey Mullier (Lund University)

Eike Schultz (Max Planck Institute for the Structure and Dynamics of Matter, Hamburg)

Christine Silberhorn (Paderborn University)

Henning Tidow (Universität Hamburg)

Charlotte Uetrecht (Heinrich Pette Institute, Leibniz Institute for Experimental Virology, Hamburg & European XFEL, Schenefeld)

Local organising committee

Robert Blick (Nanosciences)

Franz Kärtner (Photon Science)

Henning Tidow (Infection and Structural Biology)

Robin Santra and Daniela Pfannkuche (speakers of the PIER Helmholtz Graduate School)

Mirko Siemssen (coordinator PIER Helmholtz Graduate School),

Matthias Kreuzeder (DESY event management)

Table of contents

Introductory course Particle and Astroparticle Physics (A1)........ 9

Introductory courses Nanoscience (A2)........ 10

Introductory course Infection and Structural Biology (B1)........ 11

Introductory course Photon Science (B2)........ 12

Focus courses Particle and Astroparticle Physics (C1)........ 13

Focus courses Photon Science (C2)........ 14

Transferable skills (C3/D3 Group A)........ 15

Transferable skills (C4/D4, Group A)........ 16

Focus course Infection and Structural Biology (D1)........ 17

Focus course Nano Science (D2)........ 18

Poster session........ 19

List of Participants

Name		Research Field
AGARWAL	NAMAN	Photon Science
Albrecht	Steffen	Particle & Astroparticle Physics
Alharbi	Khaled	Accelerator Physics
Alizadehfanaloo	Saba	Photon Science
Alves Franca	Bruno	Infection & Structural Biology
Arling	Jan-Hendrik	Particle & Astroparticle Physics
Assalauova	Dameli	Photon Science
Assi	Benoit	Particle & Astroparticle Physics
Bahns	Immo	Accelerator Physics
Balla	Prannay	Photon Science
Bartelmann	Frederik	Theoretical Physics
Basalaev	Artem	Particle & Astroparticle Physics
Bassi	Cristian	Theoretical Physics
Batra	Gayatri	Photon Science
Baudu	Baptiste	Infection & Structural Biology
Behrooz	Milad	Photon Science
Biswas	Naireeta	Photon Science
Bosworth	Daniel	Theoretical Physics
Braun	Cora	Accelerator Physics
Breckwoldt	Niels Erwin	Theoretical Physics
Cano Vargas	Agustin	Photon Science
Cheng	Chun	Particle & Astroparticle Physics
Chopra	Pragya	Photon Science
Chuchurka	Stasis	Photon Science
Colaizzi	Lorenzo	Photon Science
Conceição	Andre	Photon Science
Creon	Anne	Infection & Structural Biology
Dai	Liwei	Nano Science
Danilov	Vladyslav	Particle & Astroparticle Physics
Dörner	Simon	Photon Science
Duarte Ruiz	Daniel	Theoretical Physics
Filatov	Oleg	Particle & Astroparticle Physics
Förger	Fynn	Photon Science
Garg	Diksha	Photon Science
Gieseler	Henry	Infection & Structural Biology
Giovannetti	Gaia	Photon Science
Grattoni	Vanessa	Accelerator Physics
Grosser	Mirco	Nano Science
Gu	Yikun	Particle & Astroparticle Physics
Guida	Alessandro	Particle & Astroparticle Physics
Harihara Sharma	Chithra	Nano Science
Henkel	Christian	Accelerator Physics
Henkel	Alessandra	Infection & Structural Biology
Höfer	Judith	Particle & Astroparticle Physics

Hoffmann	Marius	Particle & Astroparticle Physics
Hoffmann	Damian	
Huang	Haoyu	Photon Science
Iqbal	Khalid	Infection & Structural Biology
Ivanov	Nikolay	Photon Science
Jaster-Merz	Sonja	Accelerator Physics
Jin	Rui	Photon Science
Kang	Yanan	Nano Science
Karakurt	Meric Koray	Accelerator Physics
Kayanattil	Meghanad	Photon Science
Kazarian	Karina	Photon Science
Kharitonov	Konstantin	Photon Science
Kole	Abhisek	Nano Science
Krebs	Dietrich	Theoretical Physics
Kroh	Tobias	Accelerator Physics
Lahey-Rudolph	Mia	Infection & Structural Biology
Lakner	Pirmin	Nano Science
Lapkin	Dmitry	Photon Science
Laumer	Dominic	Photon Science
Lechner	Marius	Infection & Structural Biology
Liu	Yang	Nano Science
Lömker	Patrick	Photon Science
Lübke	Jannik	Photon Science
Mäkelä	Toni	Particle & Astroparticle Physics
Malek Mohamadi	Sedigheh	Photon Science
Markmann	Verena	Photon Science
Marx	Daniel	Accelerator Physics
Matthies	Christopher	Particle & Astroparticle Physics
Messner	Philipp	Accelerator Physics
Meyer	Juliane	Infection & Structural Biology
Michel	Johannes	Particle & Astroparticle Physics
Mukharamova	Nastasia	Photon Science
Music	Valerija	Photon Science
Nada	Ola	Infection & Structural Biology
Ossig	Christina	Photon Science
Paraskaki	Georgia	Accelerator Physics
Pena Rodriguez	Karla	Particle & Astroparticle Physics
Pinto	Olin	Particle & Astroparticle Physics
Prester	Andreas	Infection & Structural Biology
Radkhorrami	Yasser	Particle & Astroparticle Physics
Ranasinghe	Leonardo	Nano Science
Rauer	Patrick	Accelerator Physics
Retnakaran	Haritha	Particle & Astroparticle Physics
Rivadeneira	Pablo	Particle & Astroparticle Physics
Rokaj	Vasil	Theoretical Physics
Rossia	Alejo Nahuel	Theoretical Physics
Salman	Sarper	Photon Science
Schmirander	Thorben	Theoretical Physics

Schönberg	Arthur	Photon Science
Schubert	Kaja	Photon Science
Schwickert	David	Photon Science
Sharma	Surabhi	Particle & Astroparticle Physics
Shiwani	Shiwani	Photon Science
Silletti	Laura	Photon Science
Sobottke	Torben	Photon Science
Sokolinski	Tom	Particle & Astroparticle Physics
Stark	Ryan	Accelerator Physics
Sumfleth	Malte	Photon Science
Svidras	Henrikas	Particle & Astroparticle Physics
Teubner	Melissa	Photon Science
Tober	Steffen	Nano Science
Ullah	Najeeb	Infection & Structural Biology
Vasylieva	Olga	Nano Science
von Ahnen	Janik	Particle & Astroparticle Physics
von der Heide	Heiko	Photon Science
Wahid	Ammar Bin	Photon Science
Wang	Chang-Ming	Theoretical Physics
Wang	Lu	Photon Science
Wang	Mengying	Infection & Structural Biology
Wongel	Alicia	Particle & Astroparticle Physics
Worbs	Lena	Photon Science
yamin	Sumera	Accelerator Physics
Yang	Guang	Photon Science
Zoi	Irene	Particle & Astroparticle Physics

Programme

Monday, 23 September 2019

8:30 Registration
9:00 A1: Introductory course Particle and Astroparticle Physics (SR III)
A2: Introductory course Nanoscience Science (SR II)
10:30 *Coffee break (CFEL foyer)*
11:00 B1: Introductory course Infection and Structural Biology (SR III)
B2: Introductory course Photon Science (SR II)
12:30 *Lunch break*
14:00 C1: Focus course Particle and Astroparticle Physics (SR III)
C2: Focus course Photon Science (SR II)
C3: Presentation skills (ZOQ seminar room)
C4: Career Orientation for PhD students (group A; SR I)
15:30 *Coffee break (CFEL foyer)*
16:00 D1: Focus course Infection and Structural Biology (SR III)
D2: Focus course Nanoscience (SR II)
D3: Presentation skills (group B; ZOQ seminar room)
D4: Career Orientation (group B; SR I)
17:30 *Coffee break (CFEL foyer)*
18:00 E2 Industry talk and get-together, SR II

Tuesday, 24 September 2019

9:00 A1: Introductory course Particle and Astroparticle Physics (SR III)
A2: Introductory course Nanoscience (SR II)
10:30 *Coffee break (CFEL foyer)*
11:00 B1: Introductory course Infection and Structural Biology (SR III)
B2: Introductory course Photon Science (SR II)
12:30 *Lunch break*
14:00 C1: Focus course Particle and Astroparticle Physics (SR III)
C2: Focus course Photon Science (SR II)
C3: Presentation skills (group A; ZOQ Seminar room)
C4: Career Orientation (group A; SR I)
15:30 *Coffee break (CFEL foyer)*
16:00 D1: Focus course Infection and Structural Biology (SR III)
D2: Focus course Nanoscience (SR II)
D3: Presentation skills (group B; ZOQ Seminar room)
D4: Career Orientation (group B, SR I)
17:30 *Coffee break (CFEL foyer)*
18:00 E2: Industry talk and get-together (SR II)

Wednesday, 25 September 2019

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

B2: Introductory course Photon Science (SR III)

12:30 *Lunch break*

14:00 C1: Focus course Particle and Astroparticle Physics (SR III)
C2: Focus course Photon Science (SR II)
C3: Presentation skills (group A; ZOQ Seminar room)
C4: Career Orientation (group A; SR I)

15:30 *Coffee break (CFEL foyer)*

16:00 D1: Focus course Infection and Structural Biology (SR III)
D2: Focus course Nanoscience (SR II)
D3: Presentation skills (group B; ZOQ Seminar room)
D4: Career Orientation for PhD students (group B; building 3, SR I)

17:30 *Coffee break (CFEL foyer)*

18:00 Poster Session (CFEL foyer)

19:00 E3: BBQ (CFEL foyer)

Thursday, 26 September 2019

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

10:30 *Coffee break (CFEL foyer)*

11:00 B1: Introductory course Infection and Structural Biology (SR III)
B2: Introductory course Photon Science (SR II)

12:30 *Lunch break*

14:00 C1: Focus course Particle and Astroparticle Physics (SR III)
C2: Focus course Photon Science (SR II)
C: Presentation skills (group A; ZOQ Seminar room)
C4: Career Orientation (group A; SR I)

15:30 *Coffee break (CFEL foyer)*

16:00 D1: Focus course Infection and Structural Biology (SR III)
D2: Focus course Nanoscience (SR II)
D3: Presentation skills (group B; ZOQ Seminar room)
D4: Career Orientation (group B; SR I)

17:30 *Coffee break (CFEL foyer)*

Gudrid Moortgat-Pick (Universität Hamburg), Quantum Universe (23-26 Sep)

1. Particle Physics for Pedestrains (23 Sep)
2. Understanding mass for runners (24 Sep)
3. Accelerators and Experiments Decathlon (25 Sep)
4. Olympiques at high Precision and High energy-frontier (26 Sep)

Notes:

Francesco P. Massel (University of South-Eastern Norway, Dept. of Science and Industry systems), Nanoscience: quantum physics goes "macroscopic" (23 Sep)

We can consider the nanoscale as the interface between the world of our everyday experience and the realm of microscopic quantum phenomena. In my lecture I will give an overview of how it is possible to harness quantum mechanical properties of nanosized systems for applications and to probe into long-standing questions about the very essence of quantum mechanics.

Zlatan Aksamija (University of Massachusetts Amherst, NanoEnergy & Thermophysics (NET) Lab), Nanophononics (24 Sep)

Dissipation and thermoelectric energy conversion in nanoscale devices

Andreas K.Hüttel (Regensburg University),Clean carbon nanotubes - a perfect model system for quantum nanoelectronics (24-25 Sept)

Wrapping a single graphene sheet into a tube with perfect periodic boundary conditions, single wall carbon nanotubes provide an extraordinary electronic model system. By now we can fabricate these structures perfectly clean, and observe electronic quantum states in the unperturbed band structure of the surrounding (semi)conductor. Each carbon nanotube provides as a quantum dot a periodic system of trapped charges on its own, where the observed phenomena range from single particle physics in a potential well to complex many body phenomena. Spin-orbit coupling and valley mixing can be characterized, and connections to the detailed molecular structure can be made.

Notes:

Boris Krichel (HPI, Hamburg), Mass spectrometry goes viral – an introduction to structural MS (23 Sept)

Over the last twenty years, mass spectrometry (MS) with its ability to analyze small sample amounts with high speed and sensitivity has more and more entered the structural biology with the goal to investigate the structure and dynamics of proteins as close to their native environment as possible. The use of non-perturbing labels in hydrogen-deuterium exchange MS allows for the analysis of interactions between proteins as well as their dynamic responses to the environment. Cross-linking MS on the other hand can analyze interactions in protein complexes and identify interactions in cells. Native MS allows transferring multi-protein complexes into the gas phase and has broken boundaries to overcome size limitations, so that now even the analysis of intact virions is possible. In this presentation I will introduce the principles structural MS methods and give an overview of how they bridge the gap to other biophysical techniques, and provide valuable constraints for integrative structural modeling of protein assemblies that are inaccessible by single technique approaches.

Vadim R. Kotov (UKE/CSSB, Hamburg), Cryo-electron microscopy: the future is here (24 Sept)

Single particle electron microscopy (EM) is an interdisciplinary technique where physics, chemistry, mathematics, information technology and biology meet together to deliver unprecedented insights in molecular organization of life. Rapid development of technology, instrumentation and data processing approaches solved the challenges that seemed impossible just 5 years ago, and we are yet to discover the full potential. In this talk I will discuss the key advantages of EM in obtaining atomic structures of proteins and illustrate the narrative with exciting examples from the current literature.

Maria Garcia Alai (EMBL/CSSB, Hamburg), Protein quality control for structural biology (25 Sept)

Currently a huge amount of research time and money is wasted due to a lack of reproducibility of many scientific experiments. In cases where biological reagents such as proteins and antibodies are involved, this lack in reproducibility is often due to a bad quality of these reagents. As a group of professionals daily involved in protein production and protein characterization, we are often confronted with these irreproducibility issues in our field.

Eike Schulz (MPSD, Hamburg), Time resolved X-ray Crystallography (26 Sept)

Notes:

Franz Kärtner (DESY/ Universität Hamburg), Ultrafast Optical and X-ray Sources (23-26 Sept)

We discuss the principles of ultrashort pulse generation from the optical to the X-ray wavelength range based on laser sources, nonlinear optical processes and relativistic electron beams and some of its applications.

Notes:

Geoffrey Mullier (Lund University), Most of the things you might have wanted to know about detectors* (*But were afraid to ask) (23-25 Sept)

Notes:

Christine Silberhorn (Universität Paderborn), Quantum optics and information science in multi-dimensional systems (23-24 Sept)

Photonic quantum systems, which comprise multiple optical modes as well as highly nonclassical and sophisticated quantum states of light, have been investigated intensively invarious theoretical proposals over the last decades. The ideas cover a large range of different applications in quantum technology, spanning from quantum communication and quantum metrology to quantum simulations and quantum computing. However, the experimental implementations require advanced setups of high complexity, which poses a considerable challenge. The successful realization of controlled quantum network structures is key for the future advancement of the field. Here we present three differing approaches to overcome current limitations for the experimental implementation of multi-dimensional quantum networks: non-linear integrated quantum optics, pulsed temporal modes and time-multiplexing. Non-linear integrated quantum devices with multiple channels enable the combinations of different functionalities, such as sources and fast electro-optic modulations, on a single compact monolithic structure. Pulsed photon temporal modes are defined as field orthogonal superposition states, which span a high dimensional system. They occupy only a single spatial mode and thus they can be efficiently used in single-mode fibre communication networks. Finally, time-multiplexed quantum walks are a versatile tool for the implementation of a highly flexible simulation platform with dynamic control of the underlying graph structures and propagation properties.

References:
[1] Kai-Hong Luo, Sebastian Brauner, Christof Eigner, Polina R. Sharapova, Raimund Ricken, Torsten Meier, Harald Herrmann and Christine Silberhorn, Sci. Adv. 5, 1451 (2019)
[2] Vahid Ansari, John M. Donohue, Benjamin Brecht, and Christine Silberhorn, Optica 5, 534 (2018)
[3] B. Brecht, Dileep V. Reddy, C. Silberhorn, M. G. Raymer, Phys. Rev. X 5, 041017, (2015)
[4] Thomas Nitsche, Sonja Barkhofen, Regina Kruse, Linda Sansoni, Martin Štefaňák, Aurél Gábris, Václav Potoček, Tamás Kiss, Igor Jex and Christine Silberhorn, Sci. Adv. 4, 6444 (2018)
[5] Andreas Schreiber, Aurel Gábris, Peter P. Rohde, Kaisa Laiho, Martin Stefanak, Vaclav Potocek, Craig Hamilton, Igor Jex, Christine Silberhorn, Science 336, 55 (2012)

Eleftherios Goulielmakis (Universität Rostock), Can lasers allow us to see electrons? (25-26 Sept)

The wavelength of visible light is often assumed to impose fundamental limitations in optical microscopies and time-resolved spectroscopies of matter. In optical microscopies, it limits the spatial resolution to the nanometer scale while in time-resolved techniques it is often assumed to constrain the temporal resolution to the range of femtoseconds. In these lectures, we will discuss how recent developments in modern photonic science allow us to push both these essential frontiers.

We will study how the precision measurement and control of light fields allow us to break into the attosecond domain and to track the dynamics of electrons in real-time. We will also introduce ideas as to how the laser can enable the imaging of valence electrons in solids with picometer resolution. These capabilities bring us a few steps closer to the complete spatiotemporal visualization of the microcosm on the atomic level.

Notes:

Elena Kaufman, Presentation Skills: Vocal Power and Physical Presence (23-26 Sept)

This training is particularly designed for academics who wish to present their research in an effective, engaging way. The focus areas are on public speaking, job talks and interview techniques. Successful communication involves clarity of message, confident body language, and vocal strength.
The key to fluent public speaking is learning to relax while at the same time focusing on the audience. In these training sessions you will become aware of your weaknesses while practicing your strengths to become a more dynamic public speaker.
Where should I stand? How can I project my voice? Am I communicating my message in the best possible way? These are common concerns when giving presentations or talks in any field.

This workshop will focus on strengthening vocal power and physical presence through exercises on projection, enunciation, variation, and breath control. Relaxation techniques, physical grounding, posture awareness and gestures will also be practiced. Students will leave with a tool box of exercises and clear goals for continued improvement.

Trainer:
Elena Kaufman is the founder of Creative Communications EK where she trains academics in the soft skills of presentations, job talks, and interviews. She worked as a lecturer in English at Hamburg University (American British Institute, and Fachsprachzentrum) and teaches in companies. Elena is a trained stage actor and director.
More info: http://www.creativecommunicationsek.com/

Notes:

Diana Deterra, Career orientation for PhD students (23-26 Sept)

The training has an active workshop character and includes coaching elements, as well as methods for self analysis and reflection. The training aims to build the basis to create an individual vision and career strategy plan for every participant, based on the identification of individual resources. The process is also driven by trainer-to-participant as well as peer-to-peer consultation and inspiration.

- Motivation analysis: What makes me happy and productive?
- Value identification & reflection: What are my values?
- Which values are important for my future career?
- Identification of personal needs and resources
- Development of your professional vision
- Development of a career goal, strategy & action plan
- Communication: How to sell yourself & get your strengths across
- Networking: Analysis & how to widen and keep a supporting network
- Mission possible: Tips to enter the job-jungle

The training profits from the interaction, inspiration & creativity of the participating group members.

Trainer: Dr. Diana Deterra is a systemic management coach and has a PhD in biochemistry (Universität Hamburg). Diana has a broad industry knowledge about the service and health sector. She is familiar with the demands, processes and problems of the analytical and scientific area. Diana has some 8 years of professional experience in research institutions, as Chief Scientific Officer, and in the areas of start-ups, innovation and business development.

Notes:

Charlotte Uetrecht (HPI, Hamburg & European XFEL), Flying viruses – from biophysical to structural characterization (23 Sept)

Viruses affect basically all organisms on earth. Some are detrimental to human development, whereas those targeting pathogenic bacteria or crop pathogens can be beneficial for us. An integral part of icosahedral viruses is the capsid protein shell protecting the genome. Many copies of the capsid protein often self-assemble into shells of defined size. Low binding affinity of individual subunits allows efficient assembly and gives rise to highly stable particles. These capsids can be studied by native and hydrogen/deuterium exchange mass spectrometry (MS) in terms of stoichiometry, dynamics, assembly pathways and stability. The focus will be on isolate dependent capsid stability and size as well as glycan binding induced dynamics of noroviruses, the main cause of viral gastroenteritis. Despite the remarkable sensitivity, the structural resolution is limited in native MS. Of special interest to biology is the structural transition upon nucleation of capsid assembly. However, such transient states cannot be purified and are inaccessible for crystallography. Hard X-ray free-electron-lasers (XFELs) offer an opportunity to obtain high resolution structures of single particles. How native MS benefits single particle imaging of transient intermediates at XFELs will be illustrated. Preliminary data and implications for other applications combining native MS and X-rays will be shown, especially how soft X-rays can aid native top-down experiments.

Jan Kosinski (EMBL, Hamburg/Heidelberg, CSSB), Integrative modeling based on electron microscopy data (24- Sept)

Determining the atomic structure of macromolecular complexes is crucial for understanding their function and mechanism of action. Recently, revolutions in electron microscopy (EM) brought structures of numerous complexes at near-atomic resolution. However, many complexes do not achieve high resolution due to intrinsic structural flexibility. Moreover, technological advances in in situ electron tomography now enable generating EM maps of large complexes or even organelles in the cell, but at low resolution. Integrative structural modelling allows determining the structure of such complexes by integrating low-resolution EM data with data from other experiments, such as X-ray crystallography, NMR, SAXS or cross-linking mass spectrometry. During my talk, I will present an introduction to fitting atomic structures into EM maps and basics of integrative modelling of protein complexes. I will use examples from our own research on human nuclear pore complex and Elongator complex.

Henning Tidow (Universität Hamburg), Membrane Protein Structural Biology (25 Sep)

Sebastian Busch (MLZ Garching & HZG), Small-angle scattering for large-scale structures (26-Sept)

When molecules cannot be crystallized -- or their structure could be deformed in the process -- small-angle scattering (SAS) of neutrons and X-rays can still determine their overall size and shape on the nanometer scale. We will discuss the origin of SAS scattering, what one can learn from it, and how it is possible to make parts invisible -- and how all of this can be used for biological structure determination.

Francesco P. Massel (University of South-Eastern Norway, Dept. of Science and Industry systems), Macroscopic quantum states in optomechanics, (23 Sep)

In my lecture, I will give an introduction to the physics of optomechanical systems in the quantum regime. In particular, I will focus on the generation of quantum mechanical states for mechanical oscillators and the potential exploitation of quantum optomechanical systems in quantum information.

Zlatan Aksamija (University of Massachusetts Amherst, NanoEnergy & Thermophysics (NET) Lab, Collective and Extrinsic Effects on Phonon Transport in 2D Material (24 Sep)

Andreas K.Hüttel (Regensburg University), Nano-electromechanics of carbon nanotubes - coupling single electron effects and vibrational motion (25-26 Sept)

Carbon nanotubes are not just great electronic conductors. They are very light, with an extreme tensile strength. By now, nanotubes are used in many technological applications, ranging from bullet proof vests to surfboards or bike frames. Here, we will talk about the mechanical properties of single such molecules. The lowermost mechanical vibration mode is the transversal (or bending) mode, where the nanotube vibrates as we know it from a violin or piano string. It so far shows up in quasi-classical beam mechanics experiments, but also displays fascinating interactions between single electron effects and vibrational motion. Experiments today reach all the way to optomechanics with a single nanotube, where the vibration couples coherently to a microwave resonator field.

Notes:

Dameli Assalauova, Reconstruction of a virus structure from a single particle imaging experiment at the XFEL source (Photon Science)

D. Assalauova [1], Y. Y. Kim [1], S. Bobkov [2], M. Rose [1], K. Ayyer [3], SPI Consortium@LCLS [4], A. Aquila [4] and I. A. Vartanyants [1,5]

1 Deutsches Electronen-Synchrotron DESY, Hamburg, Germany
2 National Research Center Kurchatov Institute, Moscow, Russia
3 Center for Free Electron Laser Science CFEL, Hamburg, Germany
4 Linac Coherent Light Source LCLS at SLAC, Stanford, USA
5 National Research Nuclear University MEPhi, Moscow, Russia

Single particle imaging (SPI) is a promising area of science, which is aimed for reconstruction of the 3D structure of the nanoscale objects, including biological macromolecules, viruses, proteins and protein complexes [1]. The main advantage of this approach is that structures can be observed in native environment without any crystallization.

SPI requires performing the experiment at an x-ray free-electron laser (XFEL), which have the high intensity and large coherence length that exceeds the dimensions of the investigated particles. Many reproducible specimens of the investigated particle are injected into the x-ray beam in random orientations. Particles are destroyed during the scattering process; however, diffraction patterns corresponding to undamaged virus structure are recorded [2].

Experiments using the virus PR772 were performed at the Linac Coherent Light Source (LCLS) at SLAC, Stanford, USA in the frame of SPI consortium [3]. Previous research showed squeezed structure of the particle with the obtained resolution better than 10 nm [4]. SPI uses complex algorithms to reconstruct the structure based on the collected diffraction patterns. First, diffraction patterns of single particles are filtered out from all recorded images. In the experiment more than 200 000 diffraction patterns were collected and 1 000 were selected as single hits. After formation of 3D reciprocal space diffraction pattern with orientation determination algorithms [5], scattering phases were recovered by phase retrieval techniques [6]. After that we reconstructed the particle structure in real space with the resolution of about 13 nm. Reconstructed structure was compared with the Cryo-EM analysis of PR772 obtained at higher resolution. This comparison shows a good agreement of both techniques.

[1] R. Neutze, R. Wouts, D. van der Spoel, E. Weckert, and J. Hajdu: 'Potential for biomolecular imaging with femtosecond X-ray pulses'. Nature (2000), 406 (6797);

[2] H. N. Chapman et al.: 'Femtosecond diffractive imaging with a soft-X-ray free-electron laser', Nature Physics (2006), 2(12);

[3] A. Aquila et al.: 'The linac coherent light source single particle imaging road map', Struct Dyn. (2015), 2(4);

[4] M. Rose et al.: 'Single particle imaging without symmetry constraints at a X-ray free-electron laser'. IUCrJ (2018), 5;

[5] K. Ayyeer et al.: 'Dragonfly: an implementation of the expand-maximize–compress algorithm for single-particle imaging'. J. Appl. Crystallogr. (2016), 49 (4);

[6] J. R. Fienup: 'Phase retrieval algorithms: a comparison'. Appl. Opt. (1982), 21 (15).

Naireeta Biswas, Structural Dynamics Correlation of Peptides derived from Nups: Time-resolved X-ray Scattering and Computational Modelling (Photon Science)

Naireeta Biswas [a,b], Krishnayan Basuroya, Jakob Soltau[b], Markus Osterhoff[b], Mathias Sander[c], Matteo Levantino[c], Michael Wulff[c], Simone Techert [a, b]
[a] FS-SCS, Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany
[b] University of Göttingen, Institute for X-ray Physics, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany
[c] European Synchrotron Radiation Facility, 71 Avenue des Martyrs, 38044 Grenoble, France.

Nuclear pore complexes (NPCs) form aqueous conduits along the nuclear membrane, controlling exchange of macromolecules between the cytoplasm and the cell nucleus. The complex is built up of ~ 30 different types of proteins called as nucleoporins (Nups) which contain phenylalanine-glycine (FG) repeating motifs known as FG repeat domains. These FG domains are of various types – FG, FXFG, GLFG, etc. FG repeat domains are intrinsically disordered i.e they don't have a well defines secondary structure. The FG domains facilitate a highly selective, bidirectional passage of macromolecules through the NPCs thus forming the permeability barrier. Nucleoporins control the nucleocytoplasmic exchange in a manner where it provides a free passageway for sugars, water and ions that are within ≈ 5 nm in diameter or ≈ 30 kDa in mass, but becomes extremely restrictive to molecules that exceed these limits. However, bigger or heavier molecules those are attached to nuclear transport receptor(NTRs) as cargos are recognized by the nucleoporins and subsequently allowed to pass.
Several models for the highly selective nature of the permeability barrier of the NPCs have been proposed. According to the selective phase model, the NPC permeability barrier is constructed through cohesive meshwork of the FG domains by weak hydrophobic interactions between the phenylalanine residues. The interactions are governed by the type of FG domains and its surrounding aa composition. It has been observed that these FG domains interact with each other forming a sieve like 3D hydrogel within the central channel of the NPCs.

To get an insight in the structural dynamics of these FG Nups, we have derived a set of peptides from the nucleoporin proteins containing the FG repeat domains. We are investigating the molecular dynamics of the FG repeat domains and their interactions during the gelation process using time-resolved small/wide-angel X-ray scattering (TR-SAXS/WAXS) techniques and molecular dynamics simulation.

Erwin Agustin Cano Vargas, Timing Stability Comparison Study of RF Synthesis Techniques (Photon Science)

Cano Vargas, Erwin; Cheng, Haynes Pak Hay; Berlin, Andrej; Schiepel, Philipp; Dai, Anan; Derksen, Johann; Shafak, Kemal; Kärtner, Franz

High-precision and low-noise timing transfer from a master clock to different end stations of a free-electron laser (FEL) is an essential task*. Timing precisions ranging from few tens of femtoseconds, to sub-femtosecond are required for seeded FELs and attosecond science centers. Mode-locked lasers referenced to RF standards are commonly used as master oscillators, due to their superior stability and timing precision, depicting timing jitter in the attosecond range **. In this matter, one of the biggest challenges is to transfer the timing stability of mode-locked lasers to RF sources. Here, we compare and contrast two of the most common techniques used for laser-to-RF synthesis in FEL facilities: (i) RF signal extraction from the optical pulse train using photodiodes, and (ii) VCO-to-laser synchronization. Test setups are built to measure both the absolute phase noise of the generated RF signal and the relative timing jitter with respect to the mode-locked laser. Short-term timing jitter values varying between 10 and 100 fs are achieved for different test setups, while long term timing drift ranging to some hundreds of fs due to environmental influence are observed.

* M. Xin, K. Şafak, and F. X. Kärtner, Optica, vol. 5, no. 12, pp. 1564-1578, 2018.
** J. Kim, F. X. Kärtner, Opt. Lett., vol. 32, pp. 3519–3521, 2007.

Simon Dörner, Near-edge X-ray absorption mass spectrometry on peptides in the gas-phase: From site-specific excitation to site-selective dissociation (Photon Science)

S. Dörner[1], L. Schwob[1], K. Schubert[1], K. Atak[1], C. Bülow[2], T. Lau[2], T. Schlathölter[3], M. Timm[2], V. Zamudio-Bayer[2], X. Wang3, S. Techert1,4, S. Bari1
1 - Deutsches Elektronen-Synchrotron, Hamburg, Germany
2 - HZB, Berlin, Germany
3 - Zernike Institute for Advanced Materials, University of Groningen, The Netherlands
4 - Institute for X-ray Physics, University of Göttingen, Germany

Site-selective dissociation (SSD) of biomolecules, such as peptides, induced by photon absorption is an important key to a deeper understanding of the physics behind radiation damage in biological tissue and can further be utilized in advanced investigations on the electron dynamics in biomolecules in general. However, especially in larger peptides reliable identification of fragments emerging from site-selective dissociation is challenging because of the high total photon absorption cross section of the practically evenly distributed carbon, nitrogen and oxygen atoms across the molecule. In near-edge X-ray absorption mass spectrometry (NEXAMS) one can approach this problem by scanning fragment yields around atomic absorption edges. By comparing the obtained spectra with Density functional theory (DFT) calculated X-ray absorption spectra correlations between photon induced electronic transitions and fragmentation pathways can be revealed. This method is particularly powerful for measuring the fragment yields of sulfur-containing peptides, since sulfur only occurs is the amino acids methionine and cysteine and is therefore less abundant in peptides in general.

Following this concept, we performed a NEXAMS study on leucine enkephalin and methionine enkephalin at the carbon K-, nitrogen K-, oxygen K- and sulfur L-edge. The experiments took place at the Nanocluster trap endstation of the UE52_PGM soft X-ray beamline at the BESSY II synchrotron in Berlin. Electrospray ionization was used to introduce the peptides into the gas-phase. The mass-to-charge selected parent ions were accumulated in a cryogenic linear quadrupole ion trap and subsequently irradiated. The produced cations were analyzed by time-of-flight mass spectrometry.

The photon-energy-resolved ion yields were compared to respective DFT/ROCIS-calculated X-ray absorption spectra. The comparison allowed for an assignment of the major features in the NEXAMS spectra to certain electronic transitions. While the carbon, nitrogen and oxygen K-edge data mainly demonstrated site-specific excitations, the measurement on methionine enkephalin at the sulfur L-edge even proved site-selective dissociation upon S 2p $\rightarrow \sigma^*_{CS}$ photoexcitation for two different fragments.

Karina Kazarian, Pulsed magnetic field setup for temperature dependent dynamics studies (Photon Science)

K.Kazarian[1], J. Moore[1], A. Madsen[1]

[1] European XFEL GmbH, Holzkoppel 4, 22869 Schenefeld, Germany, karina.kazarian@xfel.eu

Studies of externally excited ultrafast magnetic dynamics in condensed matter using coherent X-ray scattering techniques are subject of interest for decades. An important challenge in time-resolved magnetic studies concerns the ground-state symmetry breaking, and monitoring the recovery back through different transients. Combination of pump excitation and the possibility of probing both structural and electronic ordering in ultrafast XFEL experiments is a crucial aspect.

For these studies a pulsed magnetic field setup was designed to be employed at the Materials Imaging and Dynamics instrument (MID) at the European XFEL, based on previous version from ESRF [1]. The system has been successfully tested at beamline P09 at Petra III (figure 1). The liquid nitrogen cooled split-pair solenoid reaches a maximum field of 15 Tesla for total pulse duration of a few ms. The bunch clock of the FEL is used to synchronize a 4.5 MHz 2D detector (AGIPD), thus scattering is collected over the duration of the field pulse or offset with respect to the field. The synchronization of a single AGIPD module and B-field has also been successfully achieved at P09. The sample is cooled in an independent helium flow cryostat which is inserted into the bore of the magnet. The flow cryostat has a temperature range from ~5 to 250 K. Recently the first tests with this setup were carried out at MID with a Si(111) crystal.
Using this setup it is planned to study field-induced dynamics of the mesoscopic structure associated with the charge-density wave (CDW) that co-exists with the spin-density wave (SDW) in antiferromagnetic chromium (Cr). There has been a lot of debate about the connection between the SDW and the CDW that has a period of half the SDW and is either due to a magnetically induced lattice distortion or a purely electronic effect based on nesting of the Fermi surface [2,3].

References

[1] - Peter J.E.M. van der Linden et al, Rev. Sci. Instrum. 79, 075104 (2008).
[2] - V.L.R. Jacques et al, Phys. Rev. B 89, 245127 (2014) .
[3] - O.G. Shpyrko et al, Nature Vol 447, 68 (2007) .

Mia Lahey-Rudolph, How To: Generate Millions of Microcrystals in Living Cells for Serial Protein Crystallography *in cellulo* (Infection & Structural Biology)

Protein crystals in living cells have been observed in all domains of life. This crystallization approach holds the possibility to grow a huge number of micron-sized protein crystals with comparable properties and of high quality in a short time. With a vision to systematically exploit the potential of *in cellulo* crystallization in living insect cells for structural biology, we (the AG Redecke at Lübeck University and DESY) are establishing a streamlined process to rapidly elucidate the structural information of *in cellulo* crystallized target proteins. There are two major challenges:

1) Depending on the recombinant protein, the fraction of crystal containing cells varies between more than 80 % and less than 1 %.

2) Changes of environmental conditions during cell lysis and crystal purification result in a loss of crystal quality.

To overcome these limitations, within the scope of my PhD project we established techniques for serial diffraction data collection from *in cellulo* grown protein crystals directly within living insect cells, using synchrotron and XFEL radiation both at RT and cryo conditions. These innovative approaches avoid crystal purification and transfer of the living, crystal-containing cells, and furthermore allow direct screening of cell cultures for successful *in cellulo* protein crystallization using the X-ray beam.

Results pave the way to a more efficient use of crystal containing insect cells as suitable targets for serial diffraction data collection at synchrotrons and XFELs in the future.

Keywords: *in cellulo*, serial crystallography, SSX, SFX

Pirmin H. Lakner, Quantification of voltage-induced anion incorporation in polypyrrole thin films by in-situ X-ray reflectivity (Nanoscience)

Pirmin H. Lakner[1,2], Manuel Brinker[3], Christoph Seitz[1], Sergey Volkov[1], Patrick Huber[3] and Thomas F. Keller[1,2]

[1] DESY NanoLab, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany
[2] Physics Department, Universität Hamburg, Germany
[3] Institute of Materials Physics and Technology, Technische Universität Hamburg-Harburg, Germany

Polypyrrole is a conducting polymer with actuatoric properties due to potential-induced ion incorporation/expulsion. Anion transport over an electrolyte-polypyrrole interface was investigated by in-situ X-ray reflectivity (XRR) and electrochemical methods. Electric potentials of -0.2 V, +0.1 V and +0.5 V (vs Ag/AgCl) were applied at an electrochemically deposited polypyrrole thin film of about 30 nm on a silicon (111) crystal. An electrolyte of 0.1 M perchloric acid was used to provide mobile perchlorate anions. X-ray reflectivity enabled a precise determination of the film thickness as well as its relative change induced by the applied electric potential. Interestingly, a significantly higher relative increase of the electron density was observed. Combining XRR and electrochemical potentiostatic analysis permits to deduce the net capacitive charge transferred from the electrolyte into the film and vice versa, depending on the integrated current while switching the electric potential. An incorporation ratio of 9.0 ± 1.2 (electrons from electrolyte to film per electron transferred from film to substrate) was determined. Since sole perchlorate anion incorporation would result in a mean incorporation ratio of 50, the difference is assigned to an inverse molecular transport from the film, e.g. the displacement of water from the cavities occupied by the perchlorate. It can therefore be concluded that an exchange of matter is taking place rather than a sole incorporation. This makes polypyrrole an electrically conductive polymer with an electrical tunable electron and therefore mass density.
Electrochemical impedance spectroscopy revealed a drastic increase in conductivity of the polypyrrole film for higher potentials due to anion incorporation, i.e. increased charge carrier density. Additional cyclic voltammetry shows a high pseudocapacity typical for polymer supercapacitors.

Keywords: polymer, X-ray reflectivity, thin film, electrochemistry, supercapacitor

Dmitry Lapkin, X-ray Nanodiffraction Studies of PbS-Cu4APc Superlattices (Photon Science)

D. Lapkin[1], N. Mukharamova[1], I.A. Zaluzhnyy[1,2], A. Meier[3], P. Frech[3], S. Lazarev[1,4], Y.Y. Kim[1], D. Assalauova[1], R. Khubbutdinov[1,2], A. Ignatenko[1], M. Sprung[1], R.P. Kurta[5], F. Schreiber[6,7], I.A. Vartanyants[1,2], and M. Scheele[3,7]

1. Deutsches Elektronen-Synchrotron DESY, Germany, e-mail: dmitry.lapkin@desy.de
2. National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Russia
3. Institute of Physical and Theoretical Chemistry, University of Tübingen, Germany
4. National Research Tomsk Polytechnic University (TPU), Russia
5. European XFEL GmbH, Germany
6. Institute of Applied Physics, University of Tübingen, Germany
7. Center for Light-Matter Interaction, Sensors & Analytics LISA+, University of Tübingen, Germany

X-ray nanodiffraction is applied to study the order in mesocrystalline superlattices of PbS nanocrystals (NCs) with organic ligands – semiconductive copper tetraaminophthalocyanine (Cu4APc). Anisotropic, facet-specific interactions between NCs invoke orientational order of them into mesocrystalline assemblies with a global angular correlation between the superlattice and the atomic lattices of NCs [1]. A detailed understanding of these correlations is expected to improve the design of NC superlattices with tailored mechanical, electric and optical properties [2].

In this work we use angular X-ray cross-correlation analysis (XCCA) [3, 4] in conjunction with a nanofocused X-ray beam to reveal local correlations in the mesocrystals [5]. The Cu4APc-containing mesocrystals were grown on substrates with preliminary formed electrodes which allowed correlating their electronic properties and structure.

We found dependence of the conductivity on the unit cell parameters and orientation of the superlattice. The XCCA of these samples revealed two major possible correlations between the atomic lattices and the superlattice which affect their structural and electronic properties. These results are very promising for controlling the properties of PbS-Cu4APc mesocrystals at the structure level depending on the preparation conditions.

References
[1] - Zaluzhnyy, I. A. et al. Quantifying Angular Correlations between the Atomic Lattice and the Superlattice of Nanocrystals Assembled with Directional Linking. Nano Letters 17, 3511–3517 (2017).
[2] - Gu, X. W. et al. Tolerance to structural disorder and tunable mechanical behavior in self-assembled superlattices of polymer-grafted nanocrystals. Proceedings of the National Academy of Sciences of the United States of America 114, 2836–2841 (2017).
[3] - Altarelli, M., Kurta, R. P. & Vartanyants, I. A. X-ray cross-correlation analysis and local symmetries of disordered systems: General theory. Phys. Rev. B 82, 104207 - (2010).
[4] - Kurta, R. P., Altarelli, M. & Vartanyants, I. A. in Advances in Chemical Physics (John Wiley & Sons, 2016), pp. 1–39.
[5] - Mukharamova N. et al. Revealing Grain Boundaries and Defect Formation in Nanocrystal Superlattices by Nanodiffraction (submitted to Nano Letters).

Jannik Lübke, Controlling nanoparticles with external fields (Photon Science)

*Jannik Lübke[1,4], Salah Awel[1,4], Armando Estillore[1], Nils Roth[1,2], Amit Samanta[1], Lena Worbs[1,2], Daniel Horke[1,4], Jochen Küpper[1,2,3,4]

*presenting author

1 Center for Free-Electron Laser Science (CFEL), Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany
2 Department of Physics, Universität Hamburg, Germany
3 Department of Chemistry, Universität Hamburg, Germany
4 The Hamburg Center for Ultrafast Imaging (CUI), Universität Hamburg, Germany

In single-particle coherent x-ray diffraction experiments, diffraction patterns are recorded from individual sample particles. To overcome the inherently small signal-to-noise ratio, large numbers of identical particles need to be controlled and guided subsequently into the small focus of free-electron lasers (FELs). We establish particle control for example via electrostatic deflection or optical guiding in tractor beams [1], ultimately aiming at delivering one nanoparticle at a time into successive FEL shots.

[1] Eckerskorn et al., Proc. SPIE 9548, 95480H1-95480H12 (2015)

Verena Markmann, Structure of Colloidal Dispersion in a Liquid Micro Jet. (Photon Science)

We study colloidal silica dispersions under high shear rates with small angle x-ray scattering (SAXS). The scientific and technological interest in a material's response to shear has increased, especially with regards to the shear thickening and shear thinning properties of some fluids. These materials show a viscosity strongly dependent on the applied shear force[1]. In order to overcome the limitations on applicable shear rates in classical rheology, our experiments were in liquid jet geometry, in which shear rates of a magnitude of $10^5\ \mathrm{s}^{-1}$ were achieved.

For our experiments we used Rayleigh micro jets. After the liquid has left the nozzle tip, the free flowing liquid will relax back into an unsheared condition[2]. Timescales for this shear cessation as well as distribution of shear induced structures across the profile of a jet were investigated in this work. We measured asymmetric intensity patterns across and along the jet and calculated the azimuthal structure factor distribution. Our analysis results in an exponential decrease of shear induced behavior along the jet. Furthermore, we could show the shear cessation's dependence on the flow rate of the jet. Structure factor changes across the jet profile were connected to varying particle concentration, confirming the development of co-flowing strings in the jet.

[1] N. Wagner and J. Brady, Phys. Today 62, 27 (2009)
[2] F. Lehmkühler, J. Phy. Chem. Lett. 8, 3581-3585 (2017)

Daniel Marx, Characterization of Ultrashort Electron Bunches at the SINBAD-ARES Linac (Accelerator Physics)

The generation of ultrashort electron bunches is an active area of research in accelerator physics. A key application of such bunches is the injection into novel accelerators with high-frequency accelerating fields, such as laser-wakefield plasma accelerators or dielectric laser accelerators. The ARES linac at the SINBAD facility at DESY, which will begin operation in late 2019, has the goal of producing bunches at particle energies of 100 MeV to 150 MeV with rms lengths down to the subfemtosecond level and charges in the picocoulomb range. This poster addresses the challenge of characterizing such bunches.

Measuring the longitudinal properties of compressed, femtosecond-long bunches with sufficient resolution is a key challenge for ARES. Two transverse deflection structures, which have the novel feature of providing a variable angle of streaking, will be installed at the end of the beamline. Detailed simulations of measurements of ARES bunches show that unprecedented resolutions may be achieved with the prospective setup, which will enable subfemtosecond bunches to be measured with high precision. A new 3D charge-density reconstruction procedure, which relies on varying the streaking angle of the deflector, is proposed and demonstrated in simulations. Simulations of reconstructions of the longitudinal phase space and slice emittance are also shown and the limitations discussed. Finally, a preliminary design of this section of the beamline is proposed based on the studies performed.

Nastasia Mukharamova, Revealing Grain Boundaries and Defect Formation in Nanocrystal Superlattices by Nanodiffraction (Photon Science)

X-ray nanodiffraction is applied to study the formation and correlation of domain boundaries in mesocrystalline superlattices of PbS nanocrystals with face-centered cubic structure. Each domain of the superlattice can be described with one of two mesocrystalline polymorphs with different orientational order. Close to a grain boundary, the lattice constant decreases and the superlattice undergoes an out-of-plane rotation, while the orientation of the nanocrystals with respect to the superlattice remains unchanged. These findings are explained with the release of stress on the expense of specific nanocrystal-substrate interactions. The fact that correlations between adjacent nanocrystals are found to survive the structural changes at most grain boundaries implies that the key to nanocrystal superlattices with macroscopic domain sizes are strengthened interactions with the substrate.

Christina Ossig, XEOL as Addition to Multi-Modal Scanning X-ray Microscopy (Nanoscience)

C. Ossig[1,2], C.Strelow[2], A. Kolditz[2], J. Siebels[2], J. Flügge[2], D. Brückner[1], A. Schropp[1], J. Hagemann[1], T. Boese[1], K. Spiers[1], J. Garrevoet[1], G. Falkenberg[1], A. Mews[2], T. Kipp[2], C. Schroer[1,2], M. Stuckelberger[1]

[1]Deutsches Elektronen-Synchrotron, D-22607 Hamburg, Germany; [2]University Hamburg, D-20146 Hamburg, Germany

Multi-modal scanning X-ray microscopy measurements are an opportunity to correlate different aspects of a device under test pixel by pixel. High beam energies around 9 to 15 keV By studying the X-ray fluorescence (XRF), the X-ray beam induced current or voltage (XBIC or XBIV) as well as ptychography the composition, electrical performance and structure, of e.g. solar cells, can be correlated.

As an addition to these multi-modal measurements X-ray excited optical luminescence (XEOL) presents itself as a fitting method. XEOL is the radiative recombination of electron-hole pairs over the bandgap in a semiconductor material. This gives information on the optical performance of the device and is therefore an excellent extension of the suite of techniques to be used.

A setup including all the above mentioned techniques is described in the setting of the P06 Micro-hutch and first results of measurements on a CIGS solar cell are shown.

Leonardo Ranasinghe, Room-temperature luminescence from droplet-etched GaAs quantum dots (Nanoscience)

L. Ranasinghe[1],*, C. Heyn[1], M. Zocher[1], R. Korneev[1] and W. Hansen[1]
[1] Center for Hybrid Nanostructures (CHyN), University of Hamburg, 22761 Hamburg, Germany
*Corresponding author: leonardo.ranasinghe@uni-hamburg.de

Photoluminescence (PL) emission from strain-free epitaxial GaAs quantum dots (QDs) in refilled AlGaAs nanoholes is studied at and close to room temperature (T_R). The nanoholes, produced by local droplet etching during molecular beam epitaxy, are filled with GaAs and capped with AlGaAs for QD generation [1]. At T = 8K, the QDs show clear excitonic peaks and nearly perfect single-photon emission [2]. However, for applications, emission at T_R is crucial. Three types of samples, with QDs of about 8 nm in height, are discussed. PL measurements were taken with laser excitation of 532 nm.
In the first sample, a single layer of low density ($2x10^7$ cm^{-2}) QDs is embedded in a thin (200 nm) $Al_{0.33}Ga_{0.67}As$ barrier. Due to the thin AlGaAs, the PL background signal from the GaAs substrate is very strong and represents a significant issue in obtaining the QDs' PL signal at T_R.
To increase the intensity of the QDs signal, the second sample has a higher QD density of $4x10^8$ cm^{-2}. Similar results to those of the first sample were obtained (Fig. 1a), but after subtraction of the GaAs background, the QD emission is clearly visible at and close to T_R (Fig. 1b and c).
To further increase the emission intensity and remove the GaAs background, the third sample consists of a stack of 5 layers of high density ($4x10^8$ cm^{-2}) QDs embedded in a thick (2.8 μm) $Al^{0.23}Ga^{0.77}As/Al^{0.69}Ga^{0.31}As/Al^{0.58}Ga^{0.42}As$ barrier layer (Fig. 2a). Study of the temperature dependence of the integrated ground-state PL, reveals a decrease of intensity by nearly three orders of magnitude when increasing T from 8K to T_R; this behaviour is modelled using a rate equation approach that considers a thermally activated escape of charge carriers from the dots (Fig. 2g). Nevertheless, as shown in Fig. 2f, the PL spectrum of this sample shows no GaAs background and a strong QD ensemble PL signal at T_R with ground-state (E_0) and up to three clear excited states (E_1, E_2 and E_3).

References
[1] C. Heyn et al., Journal of Crystal Growth, 323: 263-266 (2011).
[2] A. Küster et al., Nanoscale Research Letters, 11: 282 (2016).

Yasser Radkhorami, Reconstruction of heavy flavour jets for Higgs physics at future $e^{+}e^{-}$ colliders (Particle & Astroparticle Physics)

The reconstruction of heavy flavour jets plays an important role in precision measurements of the Higgs boson. $H \rightarrow b\bar{b}$ is the most frequently occurring decay mode of the Higgs boson. Furthermore, measuring the $H \rightarrow c\bar{c}$ decay mode will be possible for the first time at an $e^{+}e^{-}$ collider. The International Large Detector proposed for the International Linear Collider is designed for particle flow reconstruction and optimized to achieve a jet energy resolution of 3-4% for light-flavour jets. Due to harder fragmentation functions and presence of semi-leptonic decays, heavy-flavour jets are expected to behave differently. In this study, $b-$ and $c-$ jets are for the first time included in the evaluation of the jet reconstruction performance. Different strategies for correcting the $b-$ and $c-$jet energy based on the identification of leptons in the jets will be presented and their impact on the jet energy resolution will be evaluated.

Sarper Salman, Comparison of two low-noise CEP stabilization methods for an environmentally stable Yb: fiber oscillator (Photon Science)

Sarper Salman[1, 2], Yuxuan Ma1, Kutan Gürel[3], Stephane Schilt[3], Chen Li[1], Jakob Fellinger[4], Stefan Droste[5], Aline S. Mayer[4], Oliver H. Heckel[4], Thomas Südmeyer[3], Christoph M. Heyl[1, 2], Ingmar Hartl[1.]

[1] Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany
[2] Helmholtz-Institute Jena, Fröbelstieg 3, 07743 Jena, Germany
[3] Laboratoire Temps-Fréquence, Université de Neuchâtel, CH-2000 Neuchâtel, Switzerland
[4] Christian Doppler Laboratory for Mid-IR Spectroscopy and Semiconductor Optics, Faculty Center for Nano Structure Research, Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria
[5]SLAC National Accelerator Laboratory, 2575 Sand Hill Rd, Menlo Park, CA, USA
Sarper.Salman@desy.de

Abstract: We stabilize the carrier-envelope offset frequency f_0 of an all-PM Yb:fiber oscillator both via pump- and cross-gain modulation. Both methods lead to sub 200 mrad integrated f_0 phase noise (10 Hz to 1 MHz), suitable for comb spectroscopy applications.

Introduction

Recently fiber-frequency comb lasers mode-locked by amplifying non-linear loop mirrors (NALM) [1] received significant attention, since they can be constructed environmentally stable using polarization maintaining fibers [2– 4]. For demanding frequency-comb spectroscopy applications and lowest noise performance, high feedback- bandwidth for self-referenced carrier-envelope offset frequency f_0 stabilization is required. Since the bandwidth of traditional pump-power modulation-feedback is limited by the gain lifetime, fast f_0 modulation techniques based on electro-optic modulators [5],[6] have been developed. Very recently it has been shown that cross-gain modulation (XGM), where an auxiliary modulated cw-seed-laser is co-propagating with the mode locked pulse train in the gain medium and can also be used to overcome this limitation [7]. In this contribution we present a low-noise NALM Yb:fiber frequency comb laser for future XUV and MIR frequency comb spectroscopy applications. We demonstrate that with both pump-modulation and XGM in combination with lag-lead feedback-circuits sub 200 mrad integrated phase noise (10 Hz to 1 MHz) can be achieved, which enables high-coherence comb spectroscopy applications.

Experimental set-up

The experimental set-up is schematically shown in Fig.1. We use 55 cm of polarization maintaining Yb-doped gain fiber (Nufern PM-YSF-HI-HP) and pm-980 polarization maintaining single-mode fiber in a NALM set-up, an intra-cavity transmission grating pair for dispersion compensation (net cavity dispersion: approx. -0.046 ps^2) and a 10% fused fiber coupler as output coupler. The oscillator is pumped by a 976nm fiber coupled diode laser (LD2). We fiber couple a 1080 nm laser diode (estimated coupled power up to 4mW) into the orthogonal polarization of the intracavity mode-locked pulse train to the gain fiber for XGM. The oscillator pulses are amplified in a Yb-doped fiber amplifier, compressed in a transmission grating compressor and coupled into 16 cm of highly nonlinear suspended-core fiber [8] for octave spanning supercontinuum generation. The 65 MHz pulse train at the compressor output has an average power of 280 mW and a pulse duration of 108 fs. The optical spectra of compressor output (17 nm FWHM bandwidth) and supercontinuum are shown in Fig. 1b) and 1c) respectively. We use an in-line f-2f interferometer and an avalanche diode for f_0 detection. We detect f_0 with an SNR of 33 dB (100 kHz RBW). After RF filtering, amplifying and pre-scaling by a factor of 4, we generate an error-signal for feedback control using a digital phase detector. We use a fast PID loop filter for feedback control with its output used for current modulation of either the 976nm laser diode LD2 used for oscillator pumping or the 1080nm auxiliary diode laser LD1 for XGM.

Experimental results

In a first experiment we record the transfer function from diode current modulation to intracavity mode-locked pulse-train power using a vector signal analyzer. The results are shown in Fig 2a. We measure a slightly lower modulation bandwidth for XGM than [7], which might be caused by the different wavelength of the XGM diode (1080 nm vs. 1025 nm in ref. [7]). We checked that the diode laser LD1 itself can be modulated with flat amplitude and phase to at least 1 MHz. In a second experiment we stabilize fo of the oscillator by feedback-controlling one of the two laser diodes LD1 and LD2 and optimizing the lead-lag parameters of the loop filter. The in-loop fo phase noise power spectral densities (PSD) measured with a signal source analyzer (Agilent E5052) are shown in Fig 2y together with the PSD of a weakly locked fo (servo bandwidth approx. 15kHz) We measure an in-loop integrated fo phase noise of 135 mrad and 162 mrad for pump- and XGM modulation respectively (integration from 10Hz to 1MHz).

In conclusion, we demonstrated a low noise all-polarization maintaining Yb:fiber NALM frequency comb laser. We achieved tight phase locking using either pump-modulation or cross-gain modulation with an integrated f_0 phase noise of 135 mrad and 162 mrad respectively. The system is ready for amplification to enable high coherence XUV and MIR spectroscopy in the near future.

References

[1] M. E. Fermann, et al., "Nonlinear amplifying loop mirror," *Opt. Lett.* **15**, 752–754 (1990).
[2] Y. Li, et al, "Low noise, self-referenced all polarization maintaining Ytterbium fiber laser frequency comb," *Opt. Exp.* **25**, 18017 (2017).
[3] W. Hänsel, et al.,"All polarization-maintaining fiber laser architecture for robust femtosecond pulse generation," *Appl. Ph. B* **123**, 41(2017).
[4] B. Xu, et al. "Fully stabilized 750-MHz Yb: fiber frequency comb," *Opt. Express* **25**, 11910–11918 (2017).
[5] C.-C. Lee, et al., "Frequency comb stabilization with bandwidth beyond the limit of gain lifetime by an intracavity graphene electro-optic modulator," *Optics Letters* **37**, 3084–3086 (2012).
[6] W. Hänsel, et al., "Electro-optic modulator for rapid control of the carrier-envelope offset frequency," CLEO 2017, *paper SF1C.5*
[7] K. Gürel, et al., "Carrier-Envelope Offset Frequency Stabilization of a Fiber Laser by Cross Gain Modulation," *IEEE Ph. J.* **10**, 1(2018). [8] L. Dong, et al., "Highly nonlinear silica suspended core fibers," *Opt. Express,* **16**, 16423–16430 (2008).

Kaja Schubert, A gas-phase NEXAMS study on the metal active site of metalloporphyrins and metalloproteins (Photon Science)

K. Schubert[1], K. Atak[1], L. Schwob[1], S. Dörner[1], C. Bülow[2], M. Timm[2], V. Zamudio-Bayer[2], T. Lau[2] and S. Bari[1]

[1] Deutsches Elektronen-Synchrotron DESY, Hamburg
[2] Institut für Methoden und Instrumentierung der Forschung mit Synchrotronstrahlung, Helmholtz Zentrum Berlin für Materialien und Energie

Metalloporphyrins (MPs) are organometallic molecules widely found in nature and composed of a porphyrin ring (such as protoporphyrin IX) coordinating a metal ion in the ring's cavity center. Their particular electronic structure makes MPs ideally suited for a number of applications, from biological functions to the usage in electronic devices.

Two MPs of particular interest are the iron protoporphyrin IX (Fe-PPIX, heme *b*) and cobalt protoporphyrin IX (Co-PPIX). The first is found as cofactor in several proteins such as cytochrome *c* and hemoglobin and plays a key role in a variety of biological functions such as electron transfer and oxygen transport. The second is known to increase the heme oxygenase-1 activity in liver cells [1]. In addition to these natural functions, MPs have found several other applications, such as in photodynamic therapy, where MPs act as photosensitizing agents whose excitation induces cytotoxic radical and reactive oxygen production, but also as a candidate for spintronic materials when arranged in 1D nanowires [2].

The electronic structure and functional activity of metalloporphyrins are determined by the type of the metal, its oxidation and spin state as well as axial ligands around the metal center [3]. In order to understand the properties of MPs it is hence of great importance to probe the local electronic structure of the metal ion. Furthermore, performing studies in the gas phase allows taking a step further in focusing on the fundamental properties of MPs, since in comparison to condensed-phase studies, the influence of the solvent can be ruled out here.

To investigate the properties of MPs, synchrotron-based light and electrospray ionization (ESI) tandem mass-spectrometry were combined, which allows studying the relaxation processes following valence or inner-shell ionization as well as disentangling the electronic structure of gas-phase ions. Near edge X-ray absorption mass spectrometry (NEXAMS) experiments were performed at the BESSY II synchrotron facility (HZB Berlin, Germany) at the soft X-ray beamline UE52_PGM with the Nanocluster trap endstation. Ion yield spectra were recorded around the cobalt (for Co-PPIX) and iron (for Fe-PPIX) L-absorption edge, where the site-selective excitation allows to probe the metal active site. Similar measurements were performed for the heme-containing protein cytochrome *c* (12.4 kDa). The results will be presented here.

[1] E. Cable et al. Mol Cell Biochem 169, 13-20 (1997).
[2] Q. Sun, Sci Rep 5, 12772 (2015).
[3] S. A. Suchkova J Phys Conf Ser 190, 12211 (2009).

Torben Schmirander, Bychkov-Rashba Spin-Orbit Coupling effects in a multi-band tight-binding model of graphene (Theoretical Physics)

Thorben Schmirander[1)], Marta Prada[1)] and Daniela Pfannkuche[1)]

[1)] I. Institut für theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg

The description of Dirac electrons in the band structure of graphene is commonly performed using effective tight binding models [1]. These effective models use single-orbital Hamiltonians with modified hopping parameters in order to account for the influence of the higher energy orbitals in graphene. We go beyond such effective models by including d-orbitals in an atomistic tight-binding model. The inclusion of the Bychkov-Rashba spin-orbit coupling splits each of the two Dirac cones into four distinct ones [2]. When considering a finite graphene sample, edge states occur, which cross the band gap and connect the Dirac cones at the K and K' point. These edge states are the key to the topological properties of graphene, because they may exhibit the Spin Hall effect [3]. The influence of the Bychkov-Rashba spin-orbit coupling on the bulk and also the edge states dispersion relation is examined. Moreover, the winding numbers around each of the cones are computed and the resulting topological properties of graphene are discussed.

[1] van Miert, G., Juricic, V. and Morais Smith, C. Phys. Rev. B 90 195414 (2014)
[2] van Gelderen, R. and Morais Smith, C., Phys. Rev. B 81 125435 (2010)
[3] Kane, C. L . and Mele, E. J., Phys. Rev. Lett. 95, 226801 (2005)

Steffen Tober, Low temperature diffusion of isotopically labelled cations in magnetite (Nanoscience)

S.Tober[(a,b)], M. Creutzburg[(a,b)], B. Arndt[(a,b)], K. Krausert[(a,b)], S. Mattauch[(c)], S. Pütter[(c)], A. Koutsioubas[(c)], A.S. Mohd[(c)], L.Volgger[(d)], H. Hutter[(d)], H. Noei[(a)], V. Vonk[a], D. Lott [(e)], A. Stierle[(a,b)*]

[a] *Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607 Hamburg, Germany*
[b] *Universität Hamburg, Fachbereich Physik Jungiusstraße 9, 20355 Hamburg, Germany*
[c] *Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science Außenstelle am Heinz Maier-Leibnitz Zentrum, Lichtenbergstraße 1, 85747 Garching, Germany.*
[d] *Technische Universität Wien, CTA, Am Getreidemarkt 9, 1060 Vienna, Austria*
[e] *Helmholtz Zentrum Geesthacht, Max Planck Str. 1, 21502 Geesthacht, Germany*
**andreas.stierle@desy.de*

To understanding the electronic properties and catalytic activity of magnetite (Fe_3O_4), knowledge about its near surface structure is particularly important. Scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) studies of the (√2×√2)R45° reconstructed (001) surface suggested a subsurface vacancy stabilisation model for this surface, later proved by surface x-ray diffraction (SXRD) [1,2]. The surface reconstruction is reported to get lifted by formic acid adsorption at room temperature [3]. Low energy electron microscopy (LEEM) experiments under oxidising conditions showed a regrowth process of Fe_3O_4-layers on (001) surfaces [4]. These observations indicate an interesting interplay between cation vacancy formation and diffusion processes. The role of near surface cation diffusion was investigated by neutron reflectivity [5]. A 25 nm thick $^{57}Fe_3O_4$ marker layer was homoepitaxially grown on top of a (001) polished natural Fe_3O_4 single crystalline substrate by reactive molecular beam epitaxy (MBE). The lower scattering length of $^{57}Fe_3O_4$ compared to natural Fe_3O_4 results in Kiessing fringes observed by NR. Due to interfacial diffusion, the fringes faded out upon annealing in the temperature range of 500 K-700 K. A substantial mass transport was observed in the near-surface region at much lower temperatures as previously known from bulk diffusion experiments [6]. Diffusion lengths and the respective diffusion constants obtained from fitted scattering length density (SLD) profiles will be compared to the results of earlier studies on bulk Fe_3O_4 at 800 K-1600 K [6,7]. The NR results are complemented by time of flight secondary ion mass spectroscopy (TOF-SIMS) data and x-ray data characterising the structural changes of the samples during the diffusion experiments.

[1] Bliem, R. *et al. Science.* 346, 2014, 1215
[2] Arndt, B. *et al. Surf. Sci.* 653, 2016, 76
[3] Gamba, O., Arndt, B. *et al.*, 2019, submitted
[4] Nie, S. *et al.*, *J. Am. Chem. Soc.* 135, 2013, 10091
[5] Schmidt, H. *et al., Adv. Eng. Mat.* 11, 2009, 466
[6] Atkinson, A. *et al.*, *Journal of materials science*, 18, 1983, 2371
[7] Dieckmann, R., *Ber. Bunsenges. Phys. Chem.* 81, 1977, 344

Lena Worbs, Nanoparticle injectors for single particle diffractive imaging (Photon Science)

Lena Worbs[1,2], Jannik Lübke[1,2,3], Nils Roth[1,2], Armando Estillore[1], Amit Samanta[1], and Jochen Küpper[1,2,3]

[1] Center for Free-Electron Laser Science (CFEL), DESY, Hamburg, Germany
[2] Department of Physics, Universität Hamburg, Germany
[3] Centre for Ultrafast Imaging, Universität Hamburg, Germany

Single particle coherent diffractive imaging requires novel sample delivery techniques and diagnostics suitable for (biological) samples in the range of 10 to 100 nm size. One approach is the use of electrospray ionization for the aerosolization of the liquid sample,followed by an aerodynamic lens stack (ALS) to produce focused or collimated nanoparticle beams at the interaction region with an x-ray pulse.
Here, we present the optimisation of the ALS geometry by simulating the gas flow fieldwithin the ALS and calculating the particle trajectories through the flow field to predict the ALS focusing behaviour for a given particle species. Varying the geometry of the ALS results in a different focusing behaviour.
We present laboratory based characterisation techniques of the resulting particle beam for a full reconstruction of the particle beam properties, like the width of the particle beam and the velocity of the particles, using side-view imaging and light-sheet imaging.

Sumera Yamin, Study for the Alignment of Focusing Solenoid of ARES RF Gun and Effect of Misalignment of Solenoid on Emittance of Space Charge Dominated Electron Beam (Accelerator Physics)

SINBAD (Short and INnovative Bunches and Accelerators at DESY) facility will host multiple experiments relating to ultra-short high brightness beams and novel experiments with ultra-high gradient. ARES (Accelerator Research Experiment at SINBAD) LINAC is an S-band photo injector to produce such electron bunches at around 100 MeV. The LINAC will be commissioned in stages with the first stage corresponding to gun commissioning. In this paper, we present studies about the scheme adopted for the alignment of focusing solenoid for the ARES gun. The method is bench marked using ASTRA simulations and will be used for alignment of solenoids of ARES.