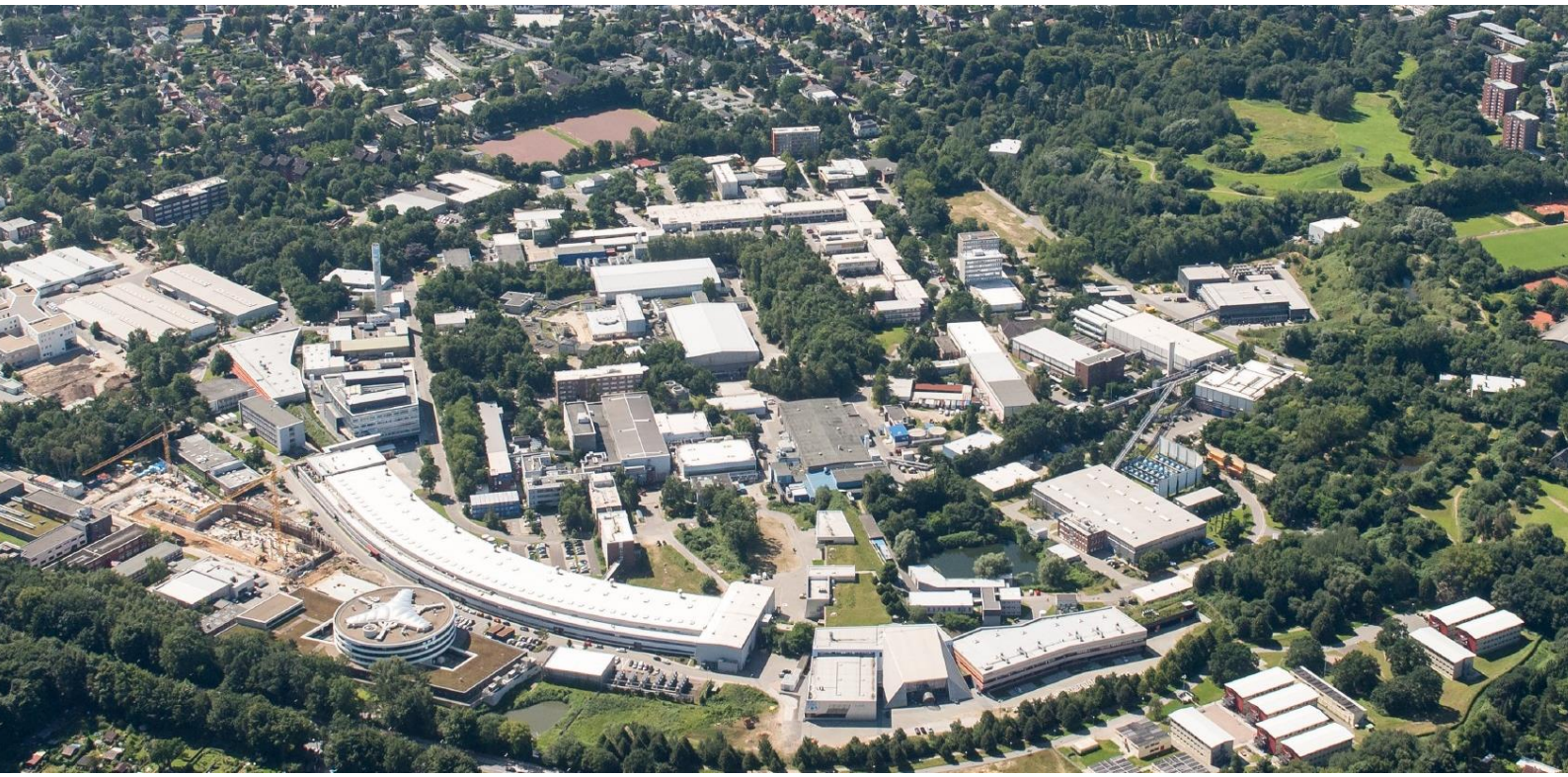

XVIII. DESY Research Course 2019

“Trends in Modern Photon Science”

27/02/2019 – 01/03/2019
DESY, Hamburg

This DESY Research course 2019 will provide a broad overview on different aspects of photon science activities of the DESY and Hamburg environment. Special attention is paid to the impact and perspectives of the latest storage ring and FEL sources, as well as lab-based methods and theory on the field.

Registration is free of charge

More information can be found on the Course’s website:

Confirmed speakers:
S. Bajt (DESY)
S. Bari (DESY)
R. Boll (European XFEL)
F. Calegari (DESY/U Hamburg)
U. Frühling (U Hamburg)
D. Pfannkuche (U Hamburg)
N. Rohringer (DESY/U Hamburg)
M. Schnell (DESY/U Kiel)
J. Simonet (U Hamburg)
S. Techert (DESY/U Göttingen)

Organizers:
Gerhard Grübel, Felix Lehmkühler
Matthias Kreuzeder

http://www.desy.de/researchcourse2019

Schedule – Research Course

27 February

13:30	*Registration*		
14:30	*Welcome*		
15:00	**Ulrike Frühling**	*U Hamburg*	Ultrafast electron dynamics studied by THz-streaking
16:00	**Daniela Pfannkuche**	*U Hamburg*	Ultrafast Quantum Chemistry with Matrix-Product-States
18:00	*Poster session*		

28 February

09:30	**Rebecca Boll**	*European XFEL*	Strongly Nonlinear Photon-Matter Interaction in X-ray Free-Electron Laser Pulses
10:30	*coffee break*		
11:00	**Sadia Bari**	*DESY*	Gas-phase biomolecules at advanced light sources
12:00	*lunch break*		
14:00	**Nina Rohringer**	*DESY & U Hamburg*	Collective decay mechanisms following saturated inner-shell x-ray excitation
15:00	*coffee break*		
15:30	**Melanie Schnell**	*DESY & U Kiel*	Following PAH astrophysics using a multi-spectroscopic approach
16:30	**Juliette Simonet**	*U Hamburg*	Magnetic phenomena for neutral atoms: Floquet engineering in optical lattices
18:30	*Dinner*		Dinner talk by **Arwen Pearson**

1 March

09:00	**Francesca Calegari**	*DESY & U Hamburg*	Attosecond Science: real-time tracking of the electron dynamics in matter
10:00	*coffee break*		
10:30	**Simone Techert**	*DESY & U Göttingen*	Guidance for Using the Time-resolution of Synchrotrons and Free Electron Lasers in Chemical Research
11:30	**Saša Bajt**	*DESY*	Some exciting new developments in X-ray optics
12:30	*Closure*		

General information

Oral sessions The oral sessions will be held in the FLASH seminar room (Bldg. 28c).

Poster session The poster session will take place in the FLASH seminar room (Bldg. 28c) on Wednesday 18:00. There will be food and drinks for all participants.

Registration The registration will start on Wednesday, 27 February 2019 at 13:30 in the lobby of the seminar room.

Social event The conference dinner will take place on Thursday, 28 February 2018 at 18:30 at the DESY canteen. There will be a Dinner presentation by Arwen Pearson (Universität Hamburg).

Meals

Breakfast
If you stay at the Mercure Hotel "Hamburg am Volkspark", breakfast will be provided there. If you stay at the DESY guest house you may have breakfast at the DESY cafeteria (opens at 07:00, building 9) at your own expenses.

Lunch
You may have lunch at the DESY canteen (building 9) and/or the Café CFEL (building 99) at your own expenses.

Supermarkets LIDL: From the main gate at Notkestrasse turn right and follow the street (700–800m).

ALDI and DENN'S BIOMARKT: From the main gate at Notkestrasse walk straight down the street "Zum Hünengrab". You will find a bakery, drugstore and other shops as well as restaurants in the vicinity

ATM You will find a cash machine in the foyer of the DESY canteen (Bldg. 9).

DESY WLAN An eduroam network is available on the DESY campus.

Guests without eduroam access will be mapped to our "Guest WLAN", it is a DESY Class-C Network which provides DHCP-Support. Before you will get internet access, you have to open your Internet browser with any requested Internet Site. Your request will be redirected to our Portal Server, a DESY form opens automatically. There you have to fill out the required fields. After submitting this form it will take about 1 minute before your requested Internet Site appears. Up to now you can use the Internet connectivity for a maximum of 90 days. **Note:** *The DESY-Guest WLAN is **unencrypted**. That means, for transferring sensitive data (e.g. passwords) secure protocols are mandatory (e.g. SSH and VPN).*

Abstracts

Ultrafast electron dynamics studied by THz-streaking

Ulrike Frühling

Universität Hamburg

Femtosecond XUV and x-ray light-sources as given by FELs or laser based HHG systems give us the opportunity to study the relaxation dynamics of highly excited atoms, molecules or clusters directly in the time domain. These systems are often investigated using experiments applying the pump-probe technique, where an intermediate state is formed with a pump-pulse and subsequently depleted with a delayed probe-pulse. THz streaking is an alternative technique. Here, the system under study is excited using fs XUV pulses and the temporal profiles of emitted electron wave-packets are probed by long wavelength (THz) light fields. In the talk the THz streaking technique will be introduced and experimental results on fs pulse metrology, electron correlations and molecular dissociations will be discussed.

Strongly Nonlinear Photon-Matter Interaction in X-ray Free-Electron Laser Pulses

Rebecca Boll

European XFEL

X-ray free-electron lasers (XFELs) have opened up unprecedented possibilities in different scientific areas. Key features of FEL radiation are the very short pulse duration and the high number of photons per pulse, leading to extreme intensities under which hitherto unknown effects in X-ray matter interaction are revealed. Multiple photoabsorptions, Auger decays, and nuclear motion occur on timescales that are comparable to the X-ray pulse duration, giving rise to effects such as resonantly-enhanced ionization, leading to extreme charge states. A detailed understanding of the atomic response on the femtosecond timescale, including strong multi-photon absorption and the interplay between electronic interactions and nuclear motion are important for the interpretation of many XFEL experiments. The Small Quantum Systems (SQS) instrument at the European XFEL started user operation in November 2018, and is dedicated to the investigation of nonlinear phenomena and ultrafast dynamics of gas-phase atoms, molecules and nanoparticles. First results from the commissioning will be presented.

Gas-phase biomolecules at advanced light sources

Sadia Bari

DESY

Investigating the interaction of light with biologically relevant molecules has gained interest for a wide variety of research fields including photochemical reactions such as light harvesting as well as radiation damage in proteins and DNA related to cutting-edge cancer treatment techniques. However, in the condensed phase, disentangling direct and indirect radiation effects is often difficult. Electrospray ionization (ESI) introduces biomolecular ions from solution into the gas phase, allowing for studies of molecular systems in a well-defined state. The coupling of ESI sources with synchrotrons and free-electron lasers (FELs) opens the way to the investigation of the electronic structure of biomolecular systems and of a fine description of their relaxation mechanisms in the VUV and soft X-ray energy range. The wide-ranging photon energy available at the synchrotrons enables systematic studies of ionization and dissociation as a function of the photon energy. Inner-shell excitations provide a localized site of energy deposition. The extremely high photon flux and fs pulse duration offered by FELs allow studying the molecular properties in intense fields. Furthermore, using the assets of FELs in a pump-probe scheme enables the study of the dynamics of charge migration and charge transfer within gas-phase biomolecules. Results will be presented of mass-spectrometric experiments at advanced light sources with different gas-phase biomolecules, e.g. proteins and oligonucleotides.

Collective decay mechanisms following saturated inner-shell x-ray excitation

Nina Rohringer

DESY & Universität Hamburg

X-ray free-electron lasers are available for experiments for almost a decade and allow for hitherto unachievable x-ray intensities on sample, reaching up to 10^{21} W/cm^2 for hard x-rays. At these intensities, the interaction probability for photo absorption of a single atom or molecule with one x-ray pulse reaches unity. Moreover, several interactions within one pulse – nonlinear x-ray mater interactions – become possible, opening the pathway to nonlinear x-ray optics. For a macroscopic ensemble of atoms, molecules, nanometer-sized clusters, or a solid the interaction with a strongly focused x-ray beam can create a macroscopic, highly excited state of matter, far from equilibrium. In particular, saturated absorption with a high-intensity x-ray pulse can result in transient states, for which every single atom in the interaction region is in a core-inverted state. This macroscopic population inversion can lead to collective radiative decay mechanisms, such as amplified spontaneous emission or superradiance. I will present recent experimental results of amplified spontaneous K-emission in transition metal compounds in solution, and superradiance of Xenon atoms following 4d-shell ionisation.

Currently we have two theoretical approaches to describe the collective, radiative relaxation dynamics of the system. The conventional approach relies on the solution of generalised Maxwell-Bloch equation – we solve the Liouville - von Neumann equation of motion for the density matrix of a few-level system coupled to a classical radiation field. In this approach, stochastic source terms have to be introduced, to mimic spontaneous decay. A more sophisticated quantum-electrodynamics approach for an atomic few-level system relies on the Heisenberg-operator equation of motion and after a series of approximations solves for the coupled equation of motion of two-point correlation function of the electronic coherences and field correlation functions. The novel approach allows us to understand the cross over from amplified spontaneous emission to super radiance. We will discuss the recent experimental results within the context of the novel theory.

Magnetic phenomena for neutral atoms: Floquet engineering in optical lattices

Juliette Simonet

Universität Hamburg

Quantum gases in optical lattices have proven to be a powerful tool for the investigation and simulation of various phenomena related to the field of many-body physics. Yet, despite its great success, some ingredients are still missing in the toolbox of quantum simulation for solid-state systems. For instance, neutral atoms owing to their zero electric charge do not couple to external gauge fields. Thus, many intriguing phenomena such as the quantum Hall effect or topological insulating phases seem to be illusive in the context of ultracold atoms in optical lattices.

Great effort has been spent to develop tools for engineering, manipulating and probing exotic quantum many-body states. In this context, time-periodic driving constitutes a powerful technique, which is subsumed under the term of Floquet engineering. The central idea is that the long-time dynamics of periodically driven quantum systems is governed by a time-independent effective Hamiltonian. Thus, appropriate driving schemes allow tailoring effective Hamiltonians that give rise to new quantum phases of matter.

Periodic driving of atoms in an optical lattice indeed enables the realization of complex-valued tunneling matrix elements with Peierls phases mimicking the effect of an external electromagnetic gauge potential. By now, diverse types of gauge potentials can be experimentally realized: Abelian gauge potentials, giving rise to synthetic electric and magnetic fields for neutral atoms as well as non-Abelian gauge potentials, such as spin-orbit coupling.

Attosecond Science: real-time tracking of the electron dynamics in matter

Francesca Calegari

DESY & Universität Hamburg

Attosecond science is nowadays a well-established research field, which offers formidable tools for the investigation and control of electronic processes. In the last few years, attosecond pulses have been used to measure the ultrafast electron dynamics occurring in atoms, molecules and solids. Electron dynamics plays a very important role in bond-formation and bond-breakage, thus determining the final chemical reactivity of a molecule. In this context, attosecond pulses can be used to attempt a control of the chemistry at the electron time scale.

In this lecture I will first introduce the basic concepts of attosecond pulse generation and characterization. I will then show recent advances and applications of attosecond technology with particular focus on the investigation of electron dynamics in biochemically relevant molecules.

Guidance for Using the Time-resolution of Synchrotrons and Free Electron Lasers in Chemical Research

Simone Techert

DESY & Universität Göttingen

Common for time-resolved x-ray experiments is the applied pump / probe scheme, often with an optical pump-laser initiating a chemical reaction whose structural time evolution is then investigated by x-ray probe pulses at various time delays. X-ray photon-in / photon-out techniques are based on x-ray diffraction, x-ray scattering or x-ray spectroscopic techniques like near edge spectroscopy or x-ray emission spectroscopy. Meanwhile x-ray spectroscopic techniques probe the local environment around specific atoms in a molecule - such as orbitals, x-ray diffraction and x-ray scattering studies reveal the structure of the bulk of periodic or disordered systems.

In the present tutorial we will give a short and comprehensive introduction into our strategy we have developed over the last 20 years for utilizing the pulsed characteristics of x-ray sources, in particular synchrotrons and free electron lasers, to gain structural dynamics information of micro- and macromolecules on their time scales of reactivity which ranges from femtoseconds to milliseconds. Method wise, we will discuss novel structural dynamics experiments in the context of time-resolved X-ray diffraction / X-ray scattering / X-ray spectroscopy.

Two detailed examples of very recent synchrotron and FEL research will be given, where ultrafast optical spectroscopy and highly brilliant, ultrafast x-ray-pulse-based structural dynamics methods have been developed as complementary tools for studying the real time structure-function relationships in (i) complex chemical reactions and of (ii) bio-mimicking opto-electronic devices and energy materials. At the end we will present a novel, pulsed-x-ray-based analysis approach for overcoming the classical description of uni- and bimolecular reactions in the traditional framework of chemistry.

References:

[1] S. Techert, et al., Ultrafast Time Structure Imprints in Complex Chemical and Biochemical Reactions, chapter 15, eds. U. Bergmann, V. Yachandra, J. Yano, Fundamentals and Application of Free Electron Lasers, Royal Chemical Society, Oxford, 301-322, (2017). doi: 10.1039/9781782624097 and references therein.

[2] S.Techert et al. Development of Ultrafast X-ray Free Electron Laser Tools in (Bio)Chemical Research, Springer Science, Berlin, in press (2019).

[3] S. Techert, Handbook for Using the Time-resolution of Synchrotrons and Free Electron Lasers in Chemical Research, J. Structural Dynamics, in press (2019).

Some exciting new developments in X-ray optics

Saša Bajt

DESY

Novel X-ray optics are essential to fully utilize bright x-ray beams from state-of-the-art synchrotron and x-ray free electron laser facilities. Due to their large penetration depth and short wavelengths hard X-rays can be used to obtain high-resolution images of samples in three dimensions without sectioning or staining. However, we are still struggling to build an atomic resolution x-ray microscope. What are the challenges to prepare x-ray lenses that meet the necessary specifications and how can we overcome them? This and the latest developments, particularly in the multilayer-based x-ray optics, will be discussed.

List of posters

Poster session

No.	Name	Title
1	ALISAUSKAS, Skirmantas	FLASH2 pump-probe laser: current status and performance
2	ARSLAN, Halil	Local Structure and Valence State of Iridium in Nanocrystalline and Amorphous Thin Film ZnO - IrO
3	BANJAFAR, Mohammadreza	Grazing-incidence x-ray scattering of surfaces upon high-intensity laser irradiation
4	BATZER, Markus	Surface Preparation of Ice Single Crystals
5	BENCHTABER, NASSIMA	TBA
6	BERMUDEZ MACIAS, Ivette Jazmin	Single shot temporal characterization at FLASH using THz Streaking
7	BISWAS, Naireeta	TBA
8	COLAIZZI, Lorenzo	A beamline for attosecond UV-pump XUV-probe experiments
9	CONCEIÇÃO, Andre	Probing nanostructural changes in tumoral breast tissue by SAXS-CT
10	DÖRNER, Simon	A comparative study on the photodissociation of two structurally similar peptides in the VUV range of 6 - 35 eV
11	FRENZEL, Lara	Anomalous Dynamics of Concentrated Silica-PNIPAm Nanogels
12	HAGEMANN, Johannes	Implementation of Propagation-Based Phase-Contrast Imaging at the P05 Nano Branch
13	HÖVELMANN, Svenja	X-Ray Reflectivity Investigation of Structure and Kinetics of Photoswitchable Lipid Monolayers
14	IVASHKO, Oleh	Charge-Stripe Order and Superconductivity in Ir1xPtxTe2
15	JAIN, Avni	TBA
16	KAGERER, Philipp	Photoelectron spectroscopy on thin Fe(Se,Te) superconductor films on Bi based topological insulators
17	KARAMATSKOS, Evangelos	Optimization of field-free alignment of molecules for imaging experiments
18	KOPULA KESAVAN, Jagadesh	Crossover in electron-gas relaxation dynamics Vs exciting photon energy in EUV-excited aluninium
19	KHARITONOV, Konstantin	Spatial characterization of the focused light at FLASH2
20	KHUBBUTDINOV, Ruslan	Coherence properties of fourth generation synchrotron sources
21	KONONIKHINA, Victoria	The disordering beta phase transformation in gamma TiAl based alloys studied by synchrotron and neutron diffraction
22	LAZARZ, John	Orientation Imaging Microscopy Using Polarized Light

23	MARKMANN, Verena	Structure of a Colloidal Dispersion in a Liquid Micro Jet
24	MIJOVILOVICH, Ana	How plants deal with metals: synchrotrons shed light on metal homeostasis
25	OSTERHOFF, Markus	Correlative Imaging: Combining X-Rays with Super-Resolution Optical Microscopy
26	PHILIPPI-KOBS, André	Ultrafast Demagnetization by Extreme Ultraviolet Light
27	ROSIGKEIT, Jan	In situ experiment for selective laser melting
28	RYSOV, Rustam	Compact hard X-ray split-and-delay line for studying ultrafast dynamics at free electron laser sources
29	SARASWATHULA, Krishna Chaitanya	High-resolution mass spectrometry and velocity map imaging for ultrafast electron dynamics in complex biomolecules
30	SCHAEFER, Julia	Electron and fluorescence spectra of a water molecule irradiated by an x-ray free-electron laser pulse
31	SCHOLZ, Maria	Multimodal 3D Microscopy: Visualize Grains in Integrated Circuits
32	SCHUBERT, Kaja	Probing the electronic structure of gas-phase heme with advanced light sources
33	SCHWOB, Lucas	Using advanced light sources to probe a single atom within gas-phase peptides and proteins
34	VASIREDDI, Ramakrishna	Microfluidic Liquid Jet systems for XFELs and Synchrotrons
35	VYŠÍN, Luděk	Dose-rate dependence of radiation damage to DNA in extreme ultraviolet, soft x-ray and x-ray spectral ranges

DESY Campus map