CUI WINTER SCHOOL 2018

5th Winter School of
The Hamburg Centre for Ultrafast Imaging

Karpacz (Poland), 26.02.-02.03.2018

The Hamburg Centre for Ultrafast Imaging

How do the elementary building blocks of nature move? Can atoms, molecules and electrons in matter be controlled and driven with precision on all length and time scales?

These questions represent some of the biggest and most exciting challenges of modern science – and the central objective of The Hamburg Centre for Ultrafast Imaging (CUI): The analysis of fundamental chemical and physical processes in Photon and Nano Science.

The scientists of CUI hope to gain profound insight into fundamental phenomena such as the mechanisms of high temperature superconductivity, the appearance of different states of magnetism or the development of ordered molecular as well as biological and mesoscopic structures. The expected insights will extend and broaden our understanding of physics, chemistry and biology and will result in new applications in medicine and novel materials for key technology areas.

Research Area A - Imaging and Control of Quantum Systems

For a full understanding of structural dynamics, one needs information on the electronic as well as the nuclear degrees of freedom. This research focus uses advanced optical imaging techniques to identify key enabling features for controlling quantum state evolution. We envisage the possibility to control chemistry along the ground state electronic surface to open up all classes of molecular systems to atomic level inspection. The system size is scaled up from small molecules to collective effects in solid state or periodic media and includes the systematic study of isolated molecules with small potential barriers separating different structures but also takes into account a variable

coupling of a system to the environment. With a detailed understanding of electronic coupling to the bath we shall be able to control coherence and degree of dissipation to the point of controlling material properties. For the case of highly correlated electron-lattice systems, this knowledge will lead to new means to control coherence and macroscopic properties with the prospect to eventually create transient superconducting states at high temperatures. The design of novel materials with unique properties is greatly aided by our capabilities to build fully controllable quantum simulators based on periodic structures formed in ultracold quantum gases. In these analog quantum processors ultracold matter is tailored to mimic magnetism and superconductivity under idealized conditions. Apart from the long range correlation effects governing material properties, there is a deep fundamental issue related to the role of quantum information transport in such highly quantized systems. To this end, we are studying the coherence properties of matter waves escaping from a macroscopic quantum object like a Bose-Einstein condensate.

Research Area B - Atomically Resolved Structural Dynamics

A particular dream experiment is to directly watch atomic motions during a chemical event, such as a bond breaking. With the advent of ultrabright electron and x-ray sources, this has become possible. Techniques such as coherent imaging will allow us to directly watch atomic motions in complex systems, such as in a biological reaction or collective dynamics in a condensed matter system. In this research area we bring together multidisciplinary expertise in laser science, structural biology, chemistry, molecular physics, and imaging science and focus on the basic underlying concepts of systems from small molecules to amino acids and to protein complexes.

Research Area C – Dynamics of Order Formation on the Nanoscale

Research Area C extends the length scale of interest from the molecular level to the nanoscale where collective effects play a defining role in material properties. The study of ultrafast ordering phenomena and nucleation events is not only crucial for understanding these materials but also for the development of tools for nanoscience. With the new X-ray light sources ordering and nucleation can be investigated down to fundamental time scales of atom mobility in solids and solution, covering even short-living transient states. Research Area C is divided into three different Research Foci which focus all on time resolved investigations of ordering phenomena on the nanoscale. RFC.1 addresses the role of transient structures in molecular liquids such as water as well as the role of structural and orientational correlations for the glass transition. In RFC.2 we study nucleation and growth processes of nanoparticles and correlate their shape and phase transformations with external triggers. The subject of RFC.3 is the study of ultrafast spin ordering processes in nanostructures under the influence of dipolar and exchange interactions.

Timetable & Program

Monday

16:00 Arrival and Welcome

16:30 Late Lunch

17:00 PhD Talks Session 1

18:00 Course Area B

20:00 Dinner

21:00 Speed Introduction

Tuesday

08:30 Course Area A

10:30 Coffee Break

11:00 PhD Talks Session 2

13:00 Lunch

14:30 Course Area B

16:30 Coffee

17:00 PhD Talks Session 3

19:00 Dinner

Wednesday

08:30 Course Area A

10:30 Coffee Break

11:00 PhD Talks Session 4

13:00 Lunch

14:30 Course Area C

16:30 Coffee

17:00 Social Science

19:00 Dinner

20:00 PhD Workshops. Speakers welcome!

Thursday

08:30 Course Area C

10:30 Coffee Break

11:00 PhD Talks Session 5

13:00 Lunch & Free Time

18:00 PhD Talks Session 6

19:00 Dinner

20:00 Discussion Forum & Feedback

Friday

08:00 Check Out

08:30 PhD Talks Session 6

10:30 Coffee Break

11:00 Gathering & Resume – Time to discuss content and format of this Winter School. What did you like? What should be improved?

12:00 Lunch

13:00 Departure to Hamburg

Lecture: Area A *(chair: Thomas Seine)*

Multi-photon interferences and higher-order photon correlations: From fundamentals quantum effects to imaging applications

Prof. Dr. Joachim von Zanthier, University Erlangen-Nürnberg

Multi-photon interferences are at the basis of a plethora of phenomena and applications in quantum optics and quantum information science, ranging from Hanbury Brown Twiss (HBT) interferometry to the Hong-Ou-Mandel effect, ghost imaging, Boson sampling or optical quantum computation. In the last years, we have investigated various aspects of multi-photon interferences, e.g., demonstrating that they can be used for quantum state engineering, to study collective effects like super- and subradiance, to generate non-local correlations violating Bell inequalities, or to improve the resolution in imaging. The latter approach, based on an extension of the HBT experiment to higher order photon correlations and originally investigated in the optical domain, has been recently transferred to the regime of soft and hard x-rays, thus establishing the field of incoherent diffractive imaging. In this lecture course I will review the basic aspects of multi-photon interferences and discuss different applications.

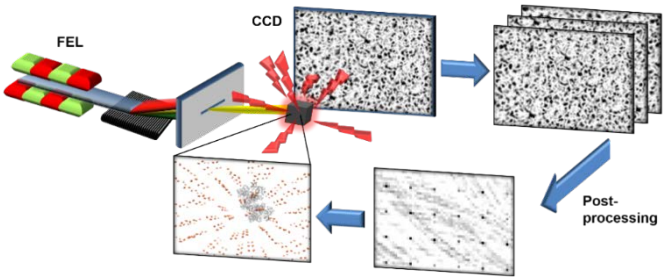

Figure 1: Illustration of incoherent dif-fraction imaging: A large number of diffraction snapshots of X-ray radiation incoherently scattered by a 3D source ensemble is recorded by a CCD; the intensity correlations of each snapshot are determined individually; averaging over many snapshots leads to a correlation pattern that – after Fourier transformation - yields the initial 3D distribution of the sources.

Lecture: Area B *(chair: Maria Katsiaflaka)*

Analyzing X-Ray Scattering Data and Modelling Biological Structures

Dr. Manfred S. Weiss, Helmholtz-Zentrum Berlin

In my lectures I will present and discuss the complete workflow of a structure determination of a protein by X-ray crystallography. The lectures will encompass all steps from the design of the construct to be analysed, cloning and protein expression, protein purification, crystallization, crystal handling, diffraction data collection and processing, diffraction data quality analysis, phase determination, model building, refinement and structure validation.

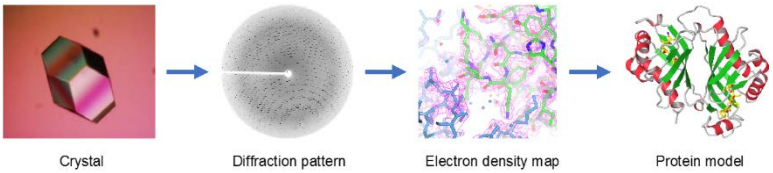

Figure 2. Workflow for protein structure determination using X-ray crystallography

Lecture: Area C *(chair: Sadegh Bakhtiarzadeh)*

Dynamics of Order Formation on the Nanoscale

Prof. Dr. Marcus Scheele, University of Tübingen

This lecture focusses on physical, chemical and dynamic aspects of the self-assembly of colloidal nanocrystals into superlattices. As such, an introduction to the thermodynamics and kinetics of synthesizing colloids in the liquid phase will be given, followed by a summary of state-of-the-art chemical strategies with a particular emphasis on the synthesis of near-monodisperse semiconductor colloids. The lecture will progress with a discussion of self-assembly techniques for colloids at the solid/air as well as the liquid/air

interface. I will highlight the structural diversity in nanocrystal assemblies as well as the role of surface molecules in tailoring the structure, and review the pivotal role of electron microscopy and X-ray scattering techniques to study these effects.

In continuation, the lecture will treat the topic of mesocrystals by detailing their unique structural features, their role in naturally occurring minerals and techniques for synthesizing these materials with colloidal nanocrystals as building blocks. It will be demonstrated how conjugated, bidendate molecules with rigid pi-systems can be utilized as linkers to facilitate the assembly of colloidal nanocrystals into mesocrystals and control their orientation. Simultaneous X-ray scattering experiments during self-assembly and surface functionalization of the nanocrystals with the molecular pi-systems allow studying these processes in-situ. Such in-situ investigations are a valuable tool to understand the various forces acting upon the colloids, which eventually determine the final structure at equilibrium.

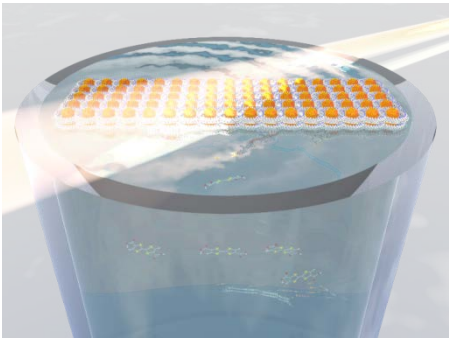

Figure 3. Idealized schematics of the self-assembly of colloidal nanocrystals at the liquid/air interface into ordered superlattices. Dispersing a molecular linker into the liquid subphase allows for simultaneous cross-linking of the nanocrystals during self-assembly. A series of X-ray scattering patterns in grazing incidence geometry serves to study the time-resolved structural evolution of the mesocrystal.

Some background literature:

(1) Boles, M. A., et al. Chem. Rev. 2016, 116, 11220–11289.
(2) Novak, J., et al. ACS Appl. Mater. Interfaces 2016, 8, 22526–22533.
(3) van der Stam, W. et al., Nano Lett. 2016, 16, 2608–2614.
(4) Weidman, M. C., et al., Nat Mater 2016, 15, 775–781.
(5) Zaluzhnyy, I., et al. Nano Lett. 2017, 17, 3511–3517.

Social Science *(chair: Markus Pfau)*

The dual use dilemma: Ethical Implications of Scientific work

Dr. Mirko Himmel, Centre for Natural Science & Peace Research Hamburg

Most if not all research disciplines the scientific show the potential to generate information, technologies, materials or knowledge that could be misused for hostile purposes. This so-called dual use dilemma can be recognized also in the life science. But in some cases, dual use research might give results that could directly be used to cause great harm. Such activities are termed dual use research of concern (DURC).

The public debate about gain-of-function experiments using artificially created airborne, human-transmissible H5N1 influenza viruses (published 2012 in Nature & Science) raised the question whether such research poses unnecessary risks for biosafety, biosecurity and public health. There was a demand by the public and by political actors for a better oversight of DURC experiments, especially in the life sciences.

The lecture will show why there is “concern” within the international security community about certain types of research. Further, we will see how publisher and scientific organizations reacted on these concerns and how that affects our daily work as scientist. At the end the leading question will be: How to deal with the immanent dual use dilemma in the life sciences? Several approaches for the mitigation of misuse of scientific achievements will be discussed.

PhD Workshop & Discussion Forum

PhD Workshops

The workshops offer the opportunity to meet with colleagues from related fields and discuss research projects in more detail. We do not want to impose any topics that should be discussed. We think more interesting discussion groups can be formed in a self-organized manner – you know best who is doing the most interesting research within CUI for you. Since this workshop should not be exclusively for PhDs try to catch one of the Postdocs or Speakers for your Session.

We will meet first in one seminar room to provide a location for the organization process. Subgroups should be formed and discuss their projects in a self-organized manner.

Discussion Forum

As CUI is running now for more than four years, we want to continue the discussion on the research cluster from our point of view. Where can we benefit from its interdisciplinarity? How could the program of the graduate school be improved? Did we make progress in developing a common language across the borders of disciplines?

In order to give a large number of people the possibility to express themselves we suggest to split up in smaller groups of 5 to 10 people. After half of the time we will meet again all together in the seminar room. One representative of each group should report the results and we will open a podium discussion. A paper with some guiding questions will be provided to facilitate the start of the discussion. Pick the two or three most interesting ones from the sheet to discuss about. You can also can discuss questions not on the sheet and present it later in the plenary part.

PhD talks

Session 1

(Monday 17:00 -18:00, chair: Marina Mutas)

- Cantaluppi, Alice - Tuning superconductivity in K3C60
- Pfäffle, Walter - Defects in semicondutor nanoparticles and their optical properties
- Pyzh, Maxim - Modeling the measurement-process of a quantum gas microscope

Session 2

(Tuesday 11:00 – 13:00, chair: Dina Sheyfer)

- Otte, Florian - Current status and future prospects of time-resolved spectroscopy at the Femtosecond X-Ray
- Jakob, Markus - THz/MIR Pulse Shaping for Ultrafast Experiments
- Bakhtiarzadeh, Sadegh - Structural studies on gas-phase using electron diffraction
- Weinkauf, Norbert - Strain induced magnetization precession in Cobalt multilayer systems
- Walther, Sophie - Time resolved coincidence measurements of interatomic Coulombic decays
- Achner, Alexander - Optical control of core hole relaxation dynamics in open shell atoms
- Gattkowski, Ellen - Structural and functional analysis of TRPM2
- Almeida, Yasser - Structural studies of rhomboid protease GlpG

Session 3

(Tuesday 17:0 0 - 19:00, chair: Maxim Pyzh)

- Bui, Thi Hanh - Empirical electronic structure correction for DFT-based calculations

- Hühnert, Jens - Calculation of the excited states of 2D-nanostructured systems
- Arnold, Caroline - Conical Intersections and Attochemistry
- Abdullah, Malik Muhammad - studying the dynamics of progressing damage in nanocrystals due to high intensity x-rays
- Köhler, Fabian - Modeling Atom-Atom Collisions Using Ultracold Atoms and the MCTDHX Method
- Minutella, Emanuele - Transient Absorption Spectroscopy on Gold Nanoparticles
- Mutas, Marina - Fluorescence lifetime imaging microscopy of fluorescent goldnanoclusters on and in cells

Session 4

(*Wednesday 11:00 – 13:00, chair: Viktor Valmispild*)

- Tang, Xiao - synthesis of CdSeCdS@SiO2@gold hybrid structures
- Ruff, Bernhard - Absolute strong-field ionization probabilities of ultracold alkali atoms
- Vakili, Mohammad - Microfluidics meets Micro-focused X-rays
- Seine, Thomas - Perspectives for in vivo Crystallization at Free Electron-Lasers
- Kesgin-Schäfer, Stephanie – New probes for (membrane) protein structure, function and dynamics
- Thomason, Chris - Towards an Optical Mass detector for High Sensitive Protein Mass Spectrometry

Session 5

(Wednesday 17:00 – 19:00, chair: Sophie Walther)

- Frenzel, Lara - Structure and Dynamics of Highly Concentrated PNIPAm Microgels
- Bourier, Felix - Mechanism of gold nanoparticle formation

- Buß, Ralph - Investigating the thickness-driven spin-reorientation transition in Co/Au multilayer films by high-resolution X-ray holographic microscopy
- Galchenko, Michael - Towards photo-switchable, gate-responsive and band-like charge transport in colloidal metal nanocluster based thin films
- Doyle, John - Photocages for X-ray Crystallography
- Sans, Marta - Improved tools for time-resolved methodologies
- Karpulevich, Anastasia - Theoretical approach to model exciton behaviour in single and coupled QDs
- Pfau, Markus - Almost Time Preserving XUV Monochromator combined with THz Streak Camera

Session 6

(Thursday 18:00 – 19:00, chair: Niclas Luick)

- Sheyfer, Dina - Structure and Dynamics in suspensions of interacting colloids studied by intensity correlation methods
- Koutentakis, Georgios - Studying ferromagnetism with few-fermion spin-flip dynamics
- Valmispild, Viktor - Electron dynamics of correlated materials
- Vasireddi, Ramakrishna - Stable flat liquid jet microfluidic system for absorption spectroscopy and reflection experiments

Session 7

(Friday 08:30 – 10:30, chair: Felix Bourier)

- Nitsche, Julius – Structural basis for activation of plasma-membrane Ca2+-ATPase by calmodulin
- Fuchs, Sebastian - Uba5 and caged-ATP: A combination to study time resolved enzymatic reactions
- Koof, Michael - Shear-induced ordering of spherical nanoparticles
- Luick, Niclas - A Homogeneous 2D Fermi gas

- Katsiaflaka, Maria - Novel techniques for thin film materials
- Ranke, Martin - Measurements of the angular energy distribution of XUV driven photoelectrons and Auger electrons in coincidence detection
- Deffner, Michael - Efficient Calculation of Electron-Phonon Coupling in Molecular Junctions

Abstracts for PhD/PostDoc Talks

Abdullah, Malik Muhammad

Studying the dynamics of progressing damage in nano-crystals due to high intensity x-rays

XFEL sources provides x-rays of high intensity which has opened new horizons for serial femotsecond crystallography and single particle imaging. In order to unreveal the structural changes induced due to high intensity x-rays pump probe experiments plays an important role. In this talk I will discuss about pump-probe experiments and a theoretical interpretation of the damage induced due to both pulses.

Achner, Alexander

Optical control of core hole relaxation dynamics in open shell atoms

To explore the relaxation dynamics of resonantly excited core-hole states of atomic iodine, we used XUV pulses from the FERMI FEL in combination with a synchronized near-infrared (NIR) laser. The ionization process was characterized by ion time of flight spectrometry. Using only XUV radiation, the resonant excitation is followed by an ultrafast resonant Auger decay leading mainly to singly and doubly charged states. Introducing the NIR laser pulses the ionization of the 4d96p resonant state is possible, causing the production of higher charge states via normal Auger process.

Almeida, Yasser

Structural studies of rhomboid protease GlpG

Rhomboid proteases are membrane proteins wide present in all living kingdoms, which perform proteolytic reactions in the lipidic environment of the cell membrane. I studied the dynamics of GlpG in solution, stabilized in detergent (fos-choline-12). We performed SAXS, SEC-SAXS, molecular dynamics simulations (MD) and functional assays, to study the dynamics of the full length protein

Arnold, Caroline

Conical Intersections and Attochemistry

With ultrashort pulses, it is now possible to create coherent superpositions of excited states of molecules by photoionization. This coherence will be affected by nuclear motion. Conical intersections, regions where non-adiabatic

couplings dominate the electron-nuclear dynamics, are abundant in polyatomic molecules. Within a 2D model system of a conical intersection, we investigate the influence of these non-adiabatic couplings on electronic coherences. We further study the possibility of attochemistry, i.e. controlling nuclear wavepacket dynamics by controlling the electronic degrees of freedom.

Bakhtiarzadeh, Sadegh

Structural studies on gas-phase using electron diffraction

To study atomic-scale structures we need photons or electrons with a wavelength of about one Angstrom and shorter. DC electron guns offer an easy and cheap apparatus compared to their X-Ray competitors, Synchrotrons and FELs, to do th9ose studies. Moreover, the guns offer shorter wavelengths which enhance the experimental resolution to a high degree fundamentally. I will report on structural studies on gas-phase samples using electron diffraction.

Bourier, Felix

Mechanism of gold nanoparticle formation

Elucidation of gold nanoparticle growth kinetics via TEM and experimental determination of rate constants and activation energies. These results get fed into particle growth simulations, which yield reasonable data for the analyzed systems and allow the extrapolation of growth kinetics for similar systems

Bui, Thi Hanh

Empirical electronic structure correction for DFT-based calculations

While Density functional theory (DFT) is extremely successful in the prediction of ground state properties and is already used as a data mining tool to design materials with certain target properties it suffers of significant deficiencies in the prediction of the electronic structure. The hope to interpret Kohn-Sham eigenvalues as quasiparticle levels to predict, e.g. optical band gaps is far from fulfilled in most semiconductors. We offer a simple correction scheme based on a modification of the non-local part of norm conserving pseudopotentials that allows for a quantitative use of the electronic structure in nanostructures. The method is implemented with the Atomic Effective Pseudopotentials AEP framework and demonstrated for various semiconductor nanostructures

Buß, Ralph

Investigating the thickness-driven spin-reorientation transition in Co/Au multilayer films by high-resolution X-ray holographic microscopy

In this talk, I will present results obtained with our x-ray holographic microscope during our recent beamtime at beamline P04 of the PETRA III storage ring. We investigated the thickness-driven spin-reorientation transition in Co/Au an Co/Pt multilayers to compare the coexistance phase of Co/Au to the canting phase of Co/Pt and study their behaviour under applied external fields.

Cantaluppi, Alice

Tuning superconductivity in K3C60

The resonant excitation of an intramolecular mode of K3C60 is capable to induce a transient superconducting-like state with a lifetime of about 2 ps. In this talk I will report the recent experimental investigation of how this exotic phase scales as external hydrostatic pressure is applied to the material.

Deffner, Michael

Efficient Calculation of Electron-Phonon Coupling in Molecular Junctions

Electron transport through individual molecules is important for many biological processes and potential technological applications. Great experimental and theoretical progress in this field in recent years also provides insight into molecular junctions under unusual (nonequilibrium) conditions. Aside from elastic processes, inelastic ones such as the excitation of spin flips or vibrations can occur. The strength of the latter is dominated by the electron-phonon coupling and is experimentally studied within the framework of inelastic electron tunneling spectroscopy using break junctions or scanning tunneling setups . The challenging aspect for theory is the sensitivity of the IET spectrum to minor changes of the molecule or the environment such as the junction geometry. Thus, efficient ways to study several junctions or structure–property relations are needed. To provide an efficient framework for calculating IET spectra, we combine the mode-tracking algorithm (an iterative subspace approach for selectively calculating eigenvectors and -modes of the Hessian matrix) as implemented in MoViPaC with our program package Artaios. We show a variety of calculated spectra, compare them with experimental data and demonstrate the capabilities of our mode–tracking approach by e.g. showing results for different numbers of gold atoms included in the electrodes.

Doyle, John

Photocages for X-ray Crystallography

In order to perform time-resolved experiments with protein crystals we need a reaction triggering mechanism. Caged compounds, or photocages, offer a possible solution for systems which are not naturally light activated. I will present the overall aims and a photochemical

Frenzel, Lara

Structure and Dynamics of Highly Concentrated PNIPAm Microgels

We study the structure and dynamics of highly concentrated core-shell nanoparticles composed by a silica core and a poly(N-isoproylacrylamide) (PNIPAm) shell. With x-ray photon correlation spectroscopy we were able to study the structural and dynamical changes of the thermoresponsive microgel which undergoes a coil-to-globule transition at a lower critical solution temperature.

Fuchs, Sebastian

Uba5 and caged-ATP: A combination to study time resolved enzymatic reactions

Uba5 is an ATP-binding protein and activator of the Ubiquitin-like protein Ufm1. In my thesis I try to use caged ATP to implement it in the protein. With this combination it will be possible to study the effects on the protein structure upon activation of ATP. Further research interest will be the changes of the conformation on the complex of Ufm1 togehter with Uba5 and caged-ATP. Recent results about nucleotide exchange and generation of microcrystals will be presented.

Galchenko, Michael

Towards photo-switchable, gate-responsive and band-like charge transport in colloidal metal nanocluster based thin films

Conventional down-scaling in the standard silicon-technology is about to reach its physical limits. To continue miniaturization and exceed Moore`s Law new designs, concepts or materials for electronic components have to be explored. Colloidal nanoparticles (NPs) offer the possibility to tune the material properties over a wide range and quantum effects can be exploited. Besides, from a cost perspective, conductive metal nanoparticle (NP) inks are promising candidates for printed electronics due to their low melting temperature and processability on large substrates. Based on this motivation and for

fundamental research aiming for single electron transistors, conductivity and switchability on single as well as on assemblies of metal NPs were investigated in the past. But charge transport in quantum confined metal NPs, especially in a thin film on which this research is focused on, was not studied in depth yet. Proceeding from a single NP to an assembly, as well new difficulties connected to the colloidal approach as a high number of tunnel barriers rise. The talk will be focussed on how these tunnel barriers can be modified by surface modification in order to achieve band-like charge transport but simultaneously maintaining the semiconducting properties of the atomically precise single NP.

Gattkowski, Ellen

Structural and functional analysis of TRPM2

The aim of my work is the functional as well as the structural characterization of the TRPM2 channel. I will present binding studies of interaction partners as well as the activating ligands to the channel. Further, I will describe the progress I made concerning the expression and purification of the protein in order to determine the structure by cryo em.

Hühnert, Jens

Calculation of the excited states of 2D-nanostructured systems

AEP's (Atomic Effective Pseudopotentials) are currently used to calculate nano dots of various materials and formatio. The goal is now to be able to calculate 2D-nanostructed systems as well.

Jakob, Markus

THz/MIR Pulse Shaping for Ultrafast Experiments

I will report about the current status of the THz/MIR pulse shaping project. The status of an femtosecond pulse shaping + characterization in the MIR spectral range is reported. An outlook on possible experiments closes the discussion

Karpulevich, Anastasia

Theoretical approach to model exciton behaviour in single and coupled QDs

Colloidal semiconductor quantum dots (QDs) can form periodic supercrystals, which can be used for various types of electronic and optical applications. The quantum mechanical atomistic calculation of the electronic properties and inter-particle interactions of experimental-size QDs remains a challenging task. We present a method within the framework of the atomic effective pseudopotential (AEP) approach. The method opens opportunities to treat

colloidal QDs of experimental size with surface passivation and band gap correction to experimental values. In the current report we demonstrate an implementation of configuration-interaction theory and trace the influence of the screening effects on the exciton lowest energies and dark-bright splitting of single and paired QDs.

Katsiaflaka, Maria

Novel techniques for thin film materials.

Ultrafast structural dynamics is a new and rapidly growig research field. A prerequisite to perform experiments on modern materials is the availability of laterally large and efficiently thin single crystalline samples. Different approaches have been tried out in order to reach these specifications.

Kesgin-Schäfer, Stephanie

New probes for (membrane) protein structure, dynamics and function

The site-specific incorporation of genetically encoded unnatural amino acids (UAAs) into (membrane) proteins via orthogonal aminoacyl-tRNA synthetase/tRNA pairs can be used to generate new probes for protein structure, dynamics and function. I seek to investigate/develop the incorporation of novel UAAs into (membrane) proteins with the aim to use them as 1) probes for (time-resolved) X-ray crystal structure determination, 2) IR-probes and 3) photo-caged probes to investigate protein dynamics and conformational changes and 4) light activated cross-link probes to study protein-protein interactions

Köhler, Fabian

Modeling Atom-Atom Collisions Using Ultracold Atoms and the MCTDHX Method

Ensembles of ultracold fermionic and bosonic atoms can be used to model a variety of different quantum systems due to their high controllability. While offering a plethora of interesting phenomena on their own, ultracold atoms, usually trapped in ultracold lattices, allow the observation of fundamental processes in systems that are otherwise hard or impossible to study. In this talk I will present my recent efforts to investigate the collisions of two atoms, modeled by ultracold atoms. As a theoretical tool the multi-configuration time-dependent hartree method for bosons (MCTDHB) and fermions is used to numerically solve the many-body Schrödinger equation. The ultimate goal of

this research is to gain a better understanding of elementary processes in such collisions (like ionization or the Auger effect).

Koof, Michael

Shear-induced ordering of spherical nanoparticles

Concentrated colloidal dispersions under shear conditions show interesting behaviour like shear thinning or thickening, that is, the reduction or increase of the dispersion's viscosity. These features are correlated to changes of the suspension's local structure which can be probed by small angle X-ray experiments. In this talk, first results of such an experiment will be presented.

Koutentakis, Georgios

Studying ferromagnetism with few-fermion spin-flip dynamics

In the widely-accepted view of the Stoner instability, ferromagnetism emerges when the repulsion between electrons with anti-oriented spins overcomes the energetic benefit of pairing them in the same single-particle state. The study of an analogue system, consisting of few spin-polarized fermionic ultracold atoms confined in a harmonic trap and subjected to a weakly-inhomogeneous transversal magnetic field, shows a behavior that deviates from the aforementioned viewpoint. In the interaction range that stable ferromagnetism is to be observed, the magnetization of the system is found to decay while the spin-spin correlator indicates that the orientation of the spins remains parallel. We discuss the quantum nature of this effect and its implications in ultracold experiments

Luick, Niclas

A Homogeneous 2D Fermi gas

Ultracold 2D Fermi gases allow to precisely characterize the interplay of reduced dimensionality and strong interactions in a quantum many-body system. So far, ultracold 2D Fermi gases have been studied in harmonic trapping potentials, which gives rise to an inhomogeneous density distribution. This complicates the interpretation of non-local quantities like correlation functions and the momentum distribution, which can only be extracted as trap-averaged quantities. In addition, the inhomogeneous density distribution reduces the chance of creating quantum phases which are predicted to exist in only small regions of the phase diagram. Here, we present our realization of an ultracold 2D Fermi gas trapped in a homogeneous disk-shaped potential.

Minutella, Emanuele

Transient Absorption Spectroscopy on Gold Nanoparticles

Experimental and theoretical aspects of transient absorption spectroscopy on gold nanoparticles.

Mutas, Marina

Fluorescence lifetime imaging microscopy of fluorescent goldnanoclusters on and in cells

We use AuNCs stabilized with mercaptoundecanoic acid (MUA-AuNCs) which show a fluorescence emission that peaks at a wavelength around 525 nm, which is in the same wavelength region as the autofluorescence of a biological cell. However, the fluorescence decay time of the MUA-AuNCs (100 ns) is much longer in comparison to the autofluorescence (3 ns). We biofunctionalize these MUA-AuNCs with biomolecules that specifically bind to the receptor expressed on the cell's membrane. To get an image of the whole cell and the bound and internalized AuNCs we use cross-sectional FLIM scans in axial direction at different heights through the cell. We distinguish between specifically bound and internalized MUA-AuNCs on and in cells by means of different FLIM methods supported by element-specific scanning electron microscopy and semi-empirical simulations.

Nitsche, Julius

Structural basis for activation of plasma-membrane Ca2+-ATPase by calmodulin

Plasma-membrane Ca2+-ATPases (PMCAs) are key regulators of Ca2+ homeostasis in eukaryotes. Belonging to the family of P-type ATPases these integral membrane proteins expel Ca2+ from the cytoplasm and thus maintain a steep Ca2+ gradient. Using a multipronged structural approach we show that activation of ACA8 by CaM involves large conformational changes. Combining ab initio and rigid body modeling of scattering data with native mass spectrometry, we present a structural model for full-length ACA8 (PMCA pump) in complex with calmodulin

Otte, Florian

Current status and future prospects of time-resolved spectroscopy at the Femtosecond X-Ray Experiment (XFEL)

A short overview of current experimental possibilities for time resolved spectroscopy at FXE (European XFEL) is given. Future plans with respect to

possible applications in our mission to resolve and understand complex chemistry are presented.

Pfäffle, Walter

Defects in semicondutor nanoparticles and their optical properties

Short recap of the method to generate the potentials I use for my calculations. Then i will show the state splitting of Mn in GaAs calculated with a post Ci-treatment method. I will also show different charged Nitrogen Vacancies defects in Diamond

Pfau, Markus

Almost Time Preserving XUV Monochromator combined with THz Streak Camera

High Harmonic Generation (HHG) is a powerful technique that gives us the opportunity of producing coherent radiation ranging from VUV to Soft X-rays, without being in need of a large accelerator facility. HHG radiation is strongly capable of investigating electron dynamics in the time domain in both atoms and molecules. In our experimental setup we combine the use of HHG radiation with an almost time-preserving monochromator for separating the various harmonics of different order. The harmonics are focused in a gas target while the XUV pulses duration stay short. In order to achieve the temporal resolution of the investigated electron dynamics we implement the use of the THz streaking technique with pulses produced by optical rectification of a Lithium Niobate Crystal. Our group has pioneered in adapting the THz- field streaking technique. In this talk some experimental data from the characterization of the radiation and some first measurements of the study of electron dynamics will be presented.

Pyzh, Maxim

Modeling the measurement-process of a quantum gas microscope

The focus of this work is to model the measurement process for a continuous, i.e. non-lattice system. The idea is to make a continuous many-body system evolve for some time, then to turn off the interactions and external potentials and finally to quickly ramp up a lattice and read out the position of particles. During a measurement process the object becomes blurred. Mathematically it means, that the image signal an experimentalists obtains, is a convolution of the true object and some point-spread function (PSF). We derive the expression for the quantum PSF and analyze its dependence on the variety of physical parameters, like the lattice depth or the ramp-up time of the lattice

Ranke, Martin

Measurements of the angular energy distribution of XUV driven photoelectrons and Auger electrons in coincidence detection

In this talk a velocity-map-imaging spectrometer with a novel gas inlet is used to analyze photoelectrons and Auger electrons in coincidence detection. Photoelectrons are generated in Xe by a high-order harmonic source which subsequently excite Auger electrons. Single shot events will be detected with a synchronized high-speed camera to analyze the angular correlation between two coupled electrons.

Ruff, Bernhard

Absolute strong-field ionization probabilities of ultracold alkali atoms

We report on precise measurements of absolute non-linear ionization probabilities obtained by exposing ultracold 87Rb atoms to the field of an ultrashort laser pulse. We have investigated both, the non-resonant and resonant strong-field response in the demanding transitional regime where the Keldysh parameter is near unity and thus ab-initio theory, based on solving time-dependent Schördingenr equation (TDSE), is required. Employing optically trapped ultracold atomic gases indeed allows retrieving absolute ionization yields since the target density is recorded simultaneously to the ionized atoms, seen as spatially resolved losses. The accurate data sets are in perfect agreement with ionization probabilities obtained by numerically solving the TDSE without any free parameters. The single outer-shell electron and the low ionization potential combined with a high polarizability compared to commonly used rare gas atoms makes alkali atoms ideal model systems for studying strong-field physics.

Sans, Marta

Improved tools for time-resolved methodologies

Synthesis of photoactive tools to trigger non-photoactive molecules for time-resolved studies.

Seine, Thomas

Perspectives for in vivo Crystallization at Free Electron-Lasers

In vivo nano-crystallization promises advantages in the reliable preparation of large amounts of small crystals for experiments at free electron-lasers (FEL).

Their usage can be conceived as a bridge between classical protein x-ray crystallography and future single particle imaging at ultra-brilliant light sources

Sheyfer, Dina

Structure and Dynamics in suspensions of interacting colloids studied by intensity correlation methods

Disordered materials, such as liquids and glasses, lack the periodicity of crystals, but are able to accommodate different local structures in the system. Revealing the local order of colloidal liquids and glasses and connect it to the dynamical properties will be a breakthrough in soft matter science. In the present study we will discuss the influence of particle concentration and interaction potential on structural and dynamical properties of polyacrylate particle suspensions. Coherent X-ray scattering in combination with X-ray Cross Correlation Analysis (XCCA) are used to study the structural properties of colloidal systems, in particular, their local orientational order and higher-order correlations. The use of X-ray Photon Correlation Spectroscopy (XPCS) reveals different dynamics in the systems.

Tang, Xiao

Synthesis of CdSeCdS@SiO2@gold hybrid structures

Inorganic semiconductor clusters have attracted much interests for their uses in the fields of photolumiscence. However, blinking as a drawback severely hinders their further application. This problem can be solved by placing the clusters in the vicinity of surface plasmon gold nanoparticles with an approproate distance. In this talk, we will introduce the technique to synthesis cluster-silica-gold hybrid structures, which rinder the clusters a suppressed blinking behavior.

Thomason, Chris

Towards an Optical Mass detector for High Sensitive Protein Mass Spectrometry

Current mass spectrometry detection methods fall short on sensitivity with high mass and low particle count. We hope to develop a detection capable of detecting a small number of particles(protein) and particularly of high mass. This is a critical limitation in current proteome studies. We have developed a nanomembrane based detector and investigate surface modification of semiconductor materials to enable sensing from mass induced vibrations coupled to electrical and optical properties. We present characterization of

different interfaces on nanomembranes explore methods application in mass sensing.

Vakili, Mohammad

Microfluidics meets Micro-focused X-rays

I work on structure determination in liquids to study fundamental chemical and physical processes such as nucleation and growth of nanoparticles and soft matter self-assembly. This includes the development of microfluidic sample environment which enables precise control over fluids on the nanoliter scale and the systematical analysis of reaction kinetics. By combining microfluidics with micro-focused X-rays, structure formation and orientational changes of polymers, colloids and proteins in laminar flow fields can be studied in situ. Here, I present microfluidic liquid jet and continuous-flow mixing devices with highly-reproducible geometric features that are suitable for time-resolved experiments at X-ray free electron lasers and synchrotron radiation facilities.

Valmispild, Viktor

Electron dynamics of correlated materials

Using time dependent dynamical mean-field theory and perturbation theory we investigate the behavior of the photoemission spectra, total energy and double occupancy of the sites, as a function of time, and on-site Coulomb repulsion U. The calculations are performed on the Bethe lattice as a benchmark and on a two-dimensional square lattice

Vasireddi, Ramakrishna

Stable flat liquid jet microfluidic system for absorption spectroscopy and reflection experiments

Our microfluidic liquid flatjet system is based on the gas dynamic virtual nozzle (GDVN) design and produces stable thin liquid sheets for solution phase X-ray experiments, i.e. transmission, absorption or reflection. Such thin liquid sheets are currently in very high demand at ultrabright photon sources, such as X-ray free electron lasers (XFELs), synchrotrons, and high-power laser facilities, due to the continuous sample replacement and they allows for a better signal to noise ratio. The gas-focusing principle reduces the flow rate considerably compared to traditional liquid sheets and, therefore, enables experiments with precious samples only available in scarce amounts. We also studied drop breakup mechanism, non-linear behavior of liquid using high speed camera while operating under atmospheric conditions making them highly relevant for

wide range of applications, for example for time resolved X-ray spectroscopic studies.

Walther, Sophie

Time resolved coincidence measurements of interatomic Coulombic decays

I will present the experimental setup for the THz-streaking experiments to measure ICD in Neon-Dimers using a Cold Target Recoil Ion Momentum Spectroscopy (COLTRIMS) detector. In the experiment XUV pulses will be superimposed with THz pulses to perform the time resolved experiments. The setup of the THz and XUV source is nearly done and I will present first tests.

Weinkauf, Norbert

Strain induced magnetization precession in Cobalt multilayer systems

We are using the transient grating excitation technique in the pump probe scheme. The strain waves induced by ultrashort intense laser pulses couple to the magnetic moments. The time-resolved measurement of the Faraday rotation and simultaneous of the diffraction gives us information about the magnetoelastic coupling. The results can be modelled by the analytical solution of the approximated Landau-Lifshitz equation. Thus strain coefficients and further material constants can be calculated

Location

Hotel Nowa Ski

ul. Mostowa 9,
58-540 Karpacz
Poland
Phone: +48757546600
Email: rezerwacja@nowaski.pl

Organizers

Lara Frenzel
DESY
FS-CXS
Notkestr. 85
22769 Hamburg
Phone: +49 (0)40 8998 2868

Stephanie Kesgin-Schäfer
University Hamburg
Institute for Biochemistry and Molecular Biology
Martin-Luther-King-Platz 6
20146 Hamburg
Phone: +49 (0)40 42838 2845

Notes

	Monday	Tuesday	Wednesday	Thursday	Friday
08:00 - 09:00					Check Out
09:00 - 10:00	Hamburg HBF to Karpacz	**Course Area A**	**Course Area A**	**Course Area C**	PhD Talks Session 7
10:00 - 11:00		Coffee Break	Coffee Break	Coffee Break	Coffee Break
11:00 - 12:00		PhD Talks Session 2	PhD Talks Session 4	PhD Talks Session 5	Gathering & Resumee
12:00 - 13:00					Lunch
13:00 - 14:00		Lunch	Lunch	Lunch & Free Time	Return to Hamburg
14:00 - 15:00					
15:00 - 16:00		**Course Area B**	**Course Area C**		
16:00 - 17:00	Short Lunch	Coffee Break	Coffee Break		
17:00 - 18:00	PhD Talks Session 1	PhD Talks Session 3	**Social Science**	PhD Talks Session 6	
18:00 - 19:00	**Course Area B**				
19:00 - 20:00		Dinner	Dinner	Dinner	
20:00 - 21:00	Dinner		PhD Workshop	Discussion Forum & Feedback	
21:00 - 22:00	Speed Introduction				

CUI THE HAMBURG CENTRE FOR ULTRAFAST IMAGING