Draft Agenda of DESY-ASU Workshop (v7.7)

28/29 April 2016, DESY Hamburg

Introduction/Motivation:

Building on the strengths of both institutions and centered on the tight cooperation between DESY and ASU on X-ray FEL applications in structural biology we will organize a workshop on 28/29 April 2016 in Hamburg. The goals are to set up and shape a future-oriented partnership between ASU and DESY by further exploring and extending the cooperation into other fields, discussing joint hiring strategies and defining roadmaps how to tap into further funding resources.

Main Parameters DESY-ASU Workshop:

- Dates:
  - Workshop: Thu/Fri, 28/29 April 2016
- Location: DESY Hamburg
- Format: Two-day workshop with different topical sessions (parallel/plenary) and wrap-up
- Participants:
  - Key scientists from ASU (~20 people)
  - DESY will invite representatives from U Hamburg and other institutes that are on campus as well as representatives from other relevant Helmholtz centers if needed for cooperation

Agenda

Wed, 27 April 2016

Arrival of ASU delegation in HAM

~17:00 Reception in the late afternoon/evening (Foyer, building 1) – Pick up of ASU delegates from Mercure Hotel at 16:45

Pre-Meeting of the Session Convenors/Chairs

Thu, 28 April 2016

08:30 Transfer of ASU Delegation from Hotel to DESY

09:00 Plenary Session I: Welcome & Opening (FLASH Seminar Room)

Welcome & Goals of the Workshop - Helmut Dosch, DESY

Overview of DESY – Helmut Dosch, DESY

Overview of ASU – William Petuskey, ASU

09:45 Plenary Session II: Overarching Scientific Themes and Opportunities at Photon Science Facilities (FLASH Seminar Room)

Speakers: John Spence (ASU), Edgar Weckert (DESY)

10:30 Coffee Break

11:00 Plenary Session III: Joint ASU & DESY Perspectives in *FELs & Structural Biology* (FLASH Seminar Room)

Speakers: Henry Chapman (DESY), Petra Fromme (ASU)

11:45 Plenary Session IV: DESY-ASU match making session - needs & demands, driven by ASU science applications/cases (FLASH Seminar Room)

Six Presentations by ASU-Speakers each 15' long: Oliver Beckstein, Dmitry Matyushov, Mariana Bertoni, Sang Heon "Dan" Shim, Giovanna Ghirlanda, Jeremy Mills

11:45 Mechanisms of membrane transport proteins from molecular simulations
Oliver Beckstein, ASU, http://becksteinlab.physics.asu.edu/

Abstract: The physiologically essential transport of small molecules and ions across the cell membrane is catalyzed by specialized integral membrane proteins. Among them the large class of active secondary transporters utilizes the free energy stored in the transmembrane electrochemical ionic gradient to power energetically-uphill transport of substrates. These transporters operate by the alternating access mechanism whereby the protein cycles between an outward facing and inward facing conformation to switch the exposure of substrate binding sites between the extracellular and the intracellular environment but the actual molecular details of these processes were poorly understood. We used a combination of molecular dynamics simulations with X-ray crystallography and functional measurements to address key questions about the transport mechanism in a nucleobase-cation symporter (NCS) and sodium-proton antiporters (NHA). While the NCS transporters undergo a rocking domain motion, the NHA were unexpectedly found to employ an elevator-like movement of domains. Together with detailed information on substrate and ion binding, we can present a molecular-level picture for key steps of the transport mechanism. Challenges remain in capturing and validating intermediate conformations in the transport cycle.

12:00 Using THz radiation for probing the evolution of interfacial water
Dmitry Matyushov, ASU, https://physics.asu.edu/content/dmitry-matyushov)

Abstract: The main area of potential interest might be the use of THz radiation to probe the evolution of interfacial water. This includes in particular water at the surface of biomolecules and lipid membranes. The advantage of time-resolved THz spectroscopy is in its ability to test millisecond and potentially longer time-scales, which are relevant for enzymes activity and allostery, but are usually outside of the time window of more precise spectroscopic techniques probing specific molecular groups. Another area of interest is the use of X-ray scattering from liquid-solid interfaces to probe the liquid structure and its modification by adsorption.

12:15 X-ray microscopy of solar absorbers for terawatt deployment
Mariana Bertoni, ASU, http://ecee.engineering.asu.edu/people/mariana-bertoni

Abstract: Our lab expertise lies in the evaluation of the defects that directly affect performance in polycrystalline absorbers for solar cells. We use multiple synchrotron-based techniques to address the effects of grain boundaries and compositional inhomogenetities across large areas of solar cell under operation. For example, we combined nano x-ray-fluorescence (nXRF) imaging with nano x-ray beam induced current (nXBIC) to provide a spot-to-spot correlation of elemental changed and charge carrier collection efficiency. To study the effects of processing conditions and various time-temperature profiles during growth we developed and in-situ stage to performed x-ray microscopy at high resolution, which is capable of heating ramps close to 200°C/min, covering a temperature range from RT to 600°C and ability to operate under corrosive atmospheres such as H2Se and H2S. --- We complement these measurements with Soft X-ray Near Edge Absorption that we normally run at beamline 10ID-1 (SM) at the Canadian Light Source (CLS), which provides the energy range and brilliance to measure the distribution of alkali metals in a scanning transmission x-ray microscopy (STXM) with a resolution of 30 nm. --- We are also interested in the use of Coherent diffraction Imaging (CDI) as a tool to investigate the stress distribution across crystallites.

12:30 Synchrotron X-ray as a tool to understand habitability of planets
Sang Heon “Dan” Shim, ASU, https://sese.asu.edu/node/1454

Abstract: Since the first observation of planets outside the solar system in 90’s, astrophysicists have found unexpected diversity among exoplanets (super-earths, water worlds, mini-neptunes, and hot jupiters): some types of exoplanets do not even exist in our solar system. On-going and near-future missions of space telescopes and ground-based telescopes demand new knowledge on planetary materials (volatiles, silicates, oxides, and metals) for analysis of astrophysical measurements and modelling of geological processes in exoplanets. Because habitability of exoplanets is of key interest from both scientific communities and general public, studying interactions between atmosphere and lithosphere and between hydrosphere and lithosphere will make immediate impacts on understanding key geochemical cycles for the habitability of exoplanets. Important techniques to be developed for such planetary materials research include generation of extreme pressure-temperature conditions and measurement of multi-phase, multi-component systems at in situ high pressure-temperature conditions. Because the samples are extremely small in size at high pressure and mapping capability is key for analysis of multi-phase samples, brilliant nanometer X-ray probes at synchrotron facilities will play key roles. In this talk, I introduce recent developments in understanding geochemical cycles in planets and discuss required techniques to solve critical issues in planetary materials science.

12:45 Protein-based hybrid catalysts for solar fuel production
Giovanna Ghirlanda, ASU, https://sms.asu.edu/giovanna_ghirlanda

Abstract: Bioinspired, protein-based molecular catalysts utilizing base metals at the active are emerging as a promising avenue to sustainable fuel production. The protein matrix modulates the intrinsic reactivity of organometallic active sites by tuning second-sphere and long-range interactions. Cobalt porphyrins are particularly attractive in this arena, as they can perform both the reduction of protons to molecular hydrogen, and the reduction of carbon dioxide to carbon monoxide and formate. These reactions can be driven either by photosensitizers, or by reductive power supplied by an electrode. Both types of reductive equivalents can be ultimately generated via solar light, thus paving the way to sustainable solar fuel production. --- The Ghirlanda group has shown that swapping Co-Protoporphyrin IX for Fe-Protoporphyrin IX in natural heme binding proteins, such as myoglobin, cytochrome c, or cytochrome b562, results in efficient catalysts for photoinduced proton reduction and CO2 reduction. Further, the activity and selectivity of wild type proteins can be modulated by a factor of 10 by exchanging the coordinating amino acids and by mutating residues in the vicinity of the active site. The observed turnover numbers (TON) for hydrogen production range between 125 and 500, and correlate well with the redox potential of the mutants. The photosensitized systems catalyze proton reduction with high efficiency even under an aerobic atmosphere, implicating its use for biotechnological applications. --- In collaboration with the Spence group, we aim to identify the electronic and molecular structure of the reaction intermediates of our protein-based catalysts during the catalytic cycle. We will use time-resolved (visible laser) pump - (X-ray) probe absorption spectroscopy to track the coordination, oxidation state and the bond-length changes in the ps time regime, with the X-ray energy tuned to the Cobalt K-edge. These measures can be performed in solution, thus providing a real-time description of the intermediates. This information will be used to redesign the catalysts and improve their activity.

13:00 The importance of structural analysis for biomolecular engineering
Jeremy Mills, ASU, https://sms.asu.edu/jeremy_mills

Abstract: Research in The Biodesign Center for Molecular Design and Biomimetics is focused on biomolecular engineering at the atomic level. Biopolymers including DNA, peptides, and proteins serve as starting points for the design of novel, functional biomolecules with properties that would not likely arise in naturally occurring organisms. Central to the efforts of researchers in the BCMDB are computational modeling tools that must constantly improve based on the success or failure of a given design challenge. Structural analysis of the predictions made by our design models plays a central role in both assessing the predictive nature of our software improving the computational methods. Recent efforts of BCMDB researchers will be discussed with emphasis on the role that structural analysis has played in these studies.

Discussions (30’)

13:45 Working Lunch for DESY/ASU Participants (Foyer FLASH Seminar Room)

15:00 – 19:00 Two Parallel/Breakout Sessions A1 and B1

Parallel Session A1: Observing/Imaging matter at micro/atomic scale (FLASH Seminar Room)

DESY: Edgar Weckert**/**Andreas Stierle/Thomas Keller (co-chairs)

ASU: Peter Crozier (co-chair), Nikhilesh Chawla, Tom Sharp, Candace Chan

Talks (15 min including discussion)

15:15 Atomic-scale imaging and spectroscopy by TEM and STEM at ASU
Thomas Sharp
School of Earth and Space Exploration, Director, LeRoy-Eyring Center for Solid State Science Director, Arizona State University

Abstract: New TEM and STEM instruments at ASU provide atomic-scale imaging and spectroscopy for the characterization of hard and soft materials. ASU and the LeRoy Eyring Center for Solid State Science have built a state-of the art facility for aberration corrected TEM/STEM that houses two probe-corrected STEM instruments (JEOL ARM 200 and the NION UltraSTEM 100) and an image-corrected environmental TEM/STEM (FEI Titan 300 ETEM). The probe-corrected STEM instruments provide 0.8-Å spatial-resolution imaging and atomic scale electron energy loss spectroscopy (EELS). The NION UltraSTEM 100 has a monochrometer that provides energy resolution as low as 12 meV. This capability allows for low-loss EELS measurements of vibrational states as well as band gap measurements at the nanometer

scale. The FEI Titan ETEM is an image-corrected TEM that allows for the atomic-resolution imaging of materials during in situ chemical reactions (See abstract by Crozier). The addition of the FEI Krios 300 cryo-EM instrument in 2016 will expand our capabilities to biological and soft materials. This instrument will be equipped with the Gatan K2 detector for rapid imaging of macromolecular structures by single-particle analysis and cryo-electron tomography. This suite of instruments is available to ASU and outside researchers as well as industrial partners.

15:30 4D Materials Science: Probing Microstructural Evolution of Metallic Materials in Real-Time

Nikhilesh Chawla (ASU)
Materials Science and Engineering, School for Engineering of Matter, Transport and Energy
Arizona State University

Advances in experimental methods, analytical techniques, and computational approaches, have now enabled the development of in situ techniques that allow us to probe the behavior of materials in real-time. The study of microstructures under an external stimulus (e.g., stress, temperature, environment) as a function of time is particularly exciting. Examples include an understanding of time-dependent deformation structures, phase transformations, compositional evolution, magnetic domains, etc. X-ray synchrotron micro and nano-tomography provides a wonderful means of characterization damage in materials non-destructively. In this talk, I will describe experiments and simulations that address the critical link between microstructure and deformation behavior of metallic materials, by using a three-dimensional (3D) virtual microstructure obtained by x-ray synchrotron tomography. The approach involves capturing the microstructure by novel and sophisticated in situ testing in an x-ray synchrotron, followed by x-ray tomography and image analysis, and 3D reconstruction of the microstructure. Case studies on fundamental precipitation evolution and deformation phenomena in aluminum alloys under cyclic loading and in a corrosive environment will be presented and discussed. New opportunities for x-ray microtomography, including lab-scale tomography and the next generation of x-ray synchrotron tomography will be highlighted, with an aim towards an integrated, complimentary, approach with the x-ray free electron laser efforts at DESY.

15:45 Hard X-Ray Microscopy with Chemical Contrast

Andreas Schropp, X-ray Nanoscience and X-ray Optics

Abstract: Hard x-ray microscopy is a powerful method for structure determination that is applied in a variety of scientific fields, such as biology, chemistry (catalysis), physics, materials science and nanotechnology. Our microscopy setup at the PETRA III beamline P06 provides access to different contrast mechanisms such as absorption spectroscopy, fluorescence and coherent x-ray diffraction. It is designed to produce focused hard x-ray beams with sizes of 50 nm (FWHM) and even smaller which allows to image structures with high resolution yielding local elemental, chemical and structural information of a specimen. Scanning coherent x-ray microscopy (ptychography) can be combined with resonant x-ray absorption methods potentially yielding local chemical information with a spatial resolution of 10 nm and even below.

16:00 Challenges and Opportunities in the Characterization of Advanced Nanomaterials for Energy Storage, Conversion, and Environmental Applications

Candace K. Chan
Materials Science and Engineering, School for Engineering of Matter, Transport and Energy
Arizona State University

Abstract: Establishing structure-property relationships is a key cornerstone of materials science. However, when materials have ill-defined structures or compositions, adopt metastable or amorphous phases, or undergo compositional/structural changes under operation conditions, obtaining detailed understanding of the origins of observed behavior can be a challenge. The development of improved materials for energy storage/conversion and environmental applications relies critically on not only the design of novel materials, but also the ability to obtain detailed fundamental understanding of materials behavior under operation conditions. This talk will highlight some example novel nanomaterials and their applications in photocatalysis, Li-ion batteries, and water treatment applications and introduce the research challenges associated with understanding them. For photocatalytic hydrogen generation and remediation of waste water, we have been interested in metal oxide photocatalysts comprising low cost, amorphous phase nanostructures and nanowires that form orthogonal hyperbranched structures in a complex, solution-based reaction. For next generation Li-ion batteries, we have studied silicon clathrates, which can electrochemically store a large number of Li+ within its cage structure without causing detectable changes to the lattice constant or local Si environment. For removal of oxoanions from waste water, understanding binding mechanisms and potential redox reactions with photocatalyst and sorbent substrates is crucial for developing better materials for water treatment.

16:15-16:35 Coffee break

16:35 Mesoscale characterization of polycrystalline bulk materials by high energy diffraction,

Ulrich Lienert, FS-PEX DESY

Abstract: As part of the PETRA III extension project the Swedish high- energy materials science beamline (P21) will become operational during 2017. The penetration power and brilliance of high-energy synchrotron radiation enables the in situ characterization of

polycrystalline bulk materials during thermomechanical processing. Real- and reciprocal space mesoscale characterization methodologies that should be available at P21 will be presented including single grain diffraction and computed tomography diffraction techniques.

16:50 Advanced Transmission Electron Microscopy Imaging and Spectroscopy of Energy Related Materials
Peter A. Crozier
Materials Science and Engineering, School for Engineering of Matter, Transport and Energy
Arizona State University
Abstract: Advanced transmission electron microscopy can provide a powerful approach for understanding structure-function relations. Aberration correction and monochromation are pushing the spatial and spectroscopic resolution to new levels providing not only atomic resolution information on structure but also on electronic and vibrational excitations. In the presence of external stimuli such as heat, gas, and photon flux, materials may undergo significant restructuring making in situ and operando observation essential to elucidate functionality. Here we briefly illustrate the application of these approaches to a variety of energy related materials for catalysts and solid oxide fuel cells. Catalytic materials are critical for chemical energy conversion processes and structure-reactivity relations on high surface area supported metal particle catalysts is complex and not well understood. Using model Ru catalysts we show that operando TEM reveals the formation of a variety of structural motifs on the catalyst surface during CO oxidation. Solar water splitting is plagued with low efficiency and materials instability issues that must be understood and resolved to develop viable technologies. We show how in situ and ex situ TEM methods can reveal surface structure, bonding configuration and morphological changes associates with catalyst deactivation. Ion conducting ceramic play important roles in solid oxide fuel cells, electrolysers etc…. The ionic conductivity is often negatively impacted by grain boundary resistance. Here we show how nanospectroscopy can be employed to reveal grain boundary segregation which can be exploited to improve ionic conductivity.

17:05 In-situ X-ray Diffraction Studies of Nanoparticle Model Catalysts,
Andreas Stierle, DESY NanoLab and University of Hamburg, Institute for Nanostructure and Solid State Physics
Abstract: The atomic structure determination of nano-objects with dimensions in the sub-100 nm regime is a formidable task for today's diffraction, imaging and scanning probe techniques. Such a detailed structural and compositional analysis is mandatory for a correlation with the nano-object's functionality e.g. as heterogeneous catalysts, magnetic storage material or light emitting device. In conventional x-ray diffraction experiments on powder samples the structural analysis is hampered by a random nanoparticle orientation and often by background scattering from the supporting material. We have therefore focused on the development of model systems based on epitaxial metal nanoparticles on single crystal oxide supports, which are stable under ambient pressure catalytic reaction conditions. Here I will present different ensemble averaging in-situ synchrotron radiation based x-ray diffraction schemes delivering quantitative information on the nanoparticle size, shape and facet surface structures under varying gas surroundings.

17:20 – 19:00 discussion of possible collaborations

Parallel Session B1: Compact X-ray and ultrafast electron sources for future applications (CFEL Seminar Room I)

DESY: Franz X. Kärtner (co-chair)

ASU: Bill Graves (co-chair)

Topics/Talks:

15.00 – 15.30: A novel noise-free x-ray laser based on electron diffraction
Bill Graves, ASU, https://www.biodesign.asu.edu/william-graves

Abstract: ASU is developing an x-ray laser that has full coherence in transverse and longitudinal planes, i.e. it does not depend on SASE gain. Instead we nanopattern the electron beam by diffracting it in a Si crystal, and then image the nanopattern into the longitudinal domain. Inverse Compton scattering is then used to produce coherent x-rays from the patterned beam. This method will produce tunable, nearly noise-free output and allows coherent control of the x-ray wavefronts including compression via optics to attosecond duration.

15.30 – 16.00: Compact X-ray and ultrafast electron sources for future applications

Scott Sayres, ASU, https://biodesign.asu.edu/scott-sayres

Abstract: Tabletop X-ray laser sources are entirely new tools for studying photochemistry and allow for fresh perspectives into the exploration of coherent electron dynamics and molecular energy transduction. A new ASU laser facility is dedicated to the production of few femtosecond to attosecond soft x-ray pulses using the principle of high harmonic generation (HHG). The bandwidth of this laser is optimized for the M-edge absorptions of transition metal elements, which are used to report on the electron motion during photochemical processes. Using tabletop x-ray transient absorption spectroscopy, we are exploring electronic wavepacket dynamics to explore details about electron correlation that are fundamentally important to understanding light-matter interaction.

16.00 – 16.30: Generation of ultra-short electron bunches

Klaus Floettmann, DESY, http://mpy.desy.de

Abstract: Electron sources providing bunch length down to the fs regime and below are of increasing interest for applications as time resolved electron diffraction or ultra-fast magnetics, but also as injectors for advanced accelerator experiments. Analytic and numerical studies demonstrate that sub-fs bunch length can be generated at low charge with simple ballistic bunching schemes if nonlinearities in the longitudinal phase space are corrected. The correction can be achieved by adding a higher harmonic rf system or by operating the rf gun in an unusual phase range in the so-called stretcher mode. The presentation will give an overview of ballistic bunching concepts and correction methods. Limits and options for ultra-short bunch generation at low energies will be discussed.

16.30 – 17.00: SINBAD - The accelerator R&D facility under construction at DESY

Barbara Marchetti, DESY, http://ard.desy.de

Abstract: Particle accelerators are used in many applications such as particle physics and radiation generation. The demand for their compactness and cost efficiency encourages the field of accelerator research and development (R&D) towards the study of novel high gradient acceleration techniques. The SINBAD facility (Short INnovative Bunches and Accelerators at Desy) is a long-term dedicated accelerator R&D facility currently under construction at DESY. Novel high gradient acceleration techniques are characterized by a short wavelength accelerating field, which require the injection of ultra-short electron bunches. The SINBAD's strategy foresees hosting multiple independent experiments combining the fields of production of ultra-short bunches for ultra-fast science and test of novel high gradient accelerating techniques.

17.00 – 17.30: Terahertz Driven Linear Acceleration and X-ray Sources

Franz Kaertner, DESY, http://ufox.cfel.de

Abstract: Theoretical and experimental advances towards a Terahertz (THz) driven accelerator and X-ray source technology are presented. The necessary strong-field THz pulses are generated with optical lasers via optical rectification and cascaded optical parametric amplification promising high optical-to-THz conversion efficiencies eventually approaching 10%. Employing accelerating frequencies two orders of magnitude higher than in conventional radio-frequency (RF) devices brings several fundamental advantages: field emission threshold for surface electric fields increases to the GV/m range, pulsed heating is strongly reduced, bunch compression to the sub-femtosecond regime at high peak currents and operation at kHz-repetition rates at room temperature. The result is a much more compact and lower cost accelerator technology tightly coupled to optical fields with intrinsic synchronization. Designs for relativistic electron guns and accelerators based on single-cycle and multi-cycle THz pulses are presented and first experimental results are discussed. Together with the implementation of an optical undulator the possibility of a completely laser driven compact Free-Electron Laser-like attosecond X-ray source arises.

17.30 – 18.00: High Energy and average power laser drivers for tabletop x-ray sources

Luis Zapata, DESY, http://ufox.cfel.de

Abstract: Energetic ~ps driving pulses are needed for the optical undulator in the planned Tabletop x-ray source we are developing as well as in the generation of single and multi-cycle THz pulses for the compact THz electron guns and LINACs. However, suitable high average power lasers are not yet available that enhance the ensuing x-ray photon flux. Particularly, the combination of short and energetic laser pulses, good beam quality, and high average power is highly demanding on the laser architecture. In developing these laser systems we are exploiting the merits of liquid nitrogen cooled Yb^{3+}:YAG and Yb^{3+}:YLF in novel large aperture composite-thin-disk geometries and placing them in image-relayed multi-pass architectures for beam quality. We have acquired empirical data at the 100 mJ level that validates our models and design methodology as we continue our efforts in scaling towards 1-J pulse energy at 1-kHz or, 1- kW average power in ps, diffraction-limited pulses.

18.00 – 19.00: Discussion

19:30 Departure for Joint DESY-ASU Dinner, Restaurant ATLAS

Contact:
Restaurant ATLAS
Schützenstr. 9a, 22761 Hamburg
Tel.: + 49 40 / 8517810
http://www.atlas.at/

Friday, 29 April 2016

08:30 Transfer of ASU Delegation from Hotel to DESY

09:00-12:30 Two Parallel Sessions A2 & B2 (and further ad-hoc meetings if needed)

Parallel Session A2: Fundamental Concepts of Matter at the Atomic Scale (FLASH Seminar Room)

Participants:

ASU: Timothy Steimle, Dmitry Matyushov, Scott Sayres, Neal Woodbury, …

DESY: Rebecca Boll, Benjamin Erk, Jochen Küpper, Tim Laarmann, Robin Santra, Sang-Kil Son, Sebastian Trippel, Jens Viefhaus, Ivan Vartaniants, …

Extern: Melanie Schnell, MPSD/CFEL, Hamburg

Convener/session chair: Jochen Küpper

Presentation times in parenthesis below start time; all speakers are kindly asked to stay within the allotted times to allow for discussions.

9:00 (10 min) - Jochen Küpper: Introduction to breakout session and context in the DESY-ASU workshop

9:10 (20 min) - Neal Woodbury: Projects at the Bio-materials interface

Abstract: Two possible areas for DESY/ASU collaboration involving interfacing biological molecules and complexes with optical and electronic materials.

a) Patterned Synthesis of Peptides for Diagnostic Chip Development (ASU Labs: Woodbury, Johnston).

Over the past six years we have developed photolithographic methods for the stepwise synthesis of peptides on silica surfaces. It is now possible to use this technology to generate peptide arrays with densities of 600,000 distinct peptides/cm^2 (1). This technology has been commercialized and used in the production of diagnostic arrays (2). A drop of blood is diluted and applied to the array. The antibodies in the blood bind to the peptides on the array in a pattern. That pattern is indicative of disease state over a very wide range of diseases from infections to chronic diseases such as cancer (1,3). Currently, the antibody binding information is read optically by using a fluorescently labeled secondary antibody that recognizes, e.g. IgG. It would be of considerable value to move to electronic readers. The challenges lie in the number of elements that need to be read (currently 130,000), the close spatial proximity of measurement elements (currently 14 micron on center), and the required sensitivity of signal detection.

b) Interfacing Biophotonic Systems with Electronic Materials (ASU Labs: Woodbury, Seo, Yan)

We have recently demonstrated that it is possible to interface photosynthetic bacterial reaction centers with porous, transparent antimony doped tin oxide electrodes or with modified reduced graphene oxide electrodes and generate photocurrents in the microamp per cm^2 range (4,5). These systems use light to generate a soluble 2-electron carrier (a quinone in this case) which can be involved in subsequent 2-electron redox chemistry. The system can be controlled either by light or the potential of the working electrode. Several areas of research are underway. First, we are replacing the bacterial reaction centers with plant PS1 reaction centers that are capable of generating reduced nicotinamide adenine dinucleotide substrates which can be directly used in nanoscale redox circuits previously developed (6,7). Second, we are adding antenna molecules or complexes to the reaction center to increase the overall absorbance cross section of the system (8). Third, we would like to explore miniaturization of the system to avoid the slow diffusion between the reaction center and the counter electrode or the redox target.

References

1. Legutki, J.B., et al., *Scalable High-Density Peptide Arrays for Comprehensive Health Monitoring.* Nature Communications, 2014. **5**: p. 4785.

2. www.healthtell.com
3. Stafford, P., et al., *Immunosignature system for diagnosis of cancer.* Proc Natl Acad Sci U S A, 2014. **111**(30): p. E3072-80.
4. Submitted to the Proc Natl Acad Sci
5. Submitted to the J Am Chem Soc
6. Fu, J., et al., *Multi-enzyme complexes on DNA scaffolds capable of substrate channeling with an artificial swinging arm.* Nature Nanotechnology, 2014, 9, 531-536
7. Liu, M., et al., *A DNA tweezer-actuated enzyme nanoreactor*. Nature Comm, 2013, DOI: 10.1038/ncomms3127
8. Dutta, P.K., et al., *A DNA-Directed Light-Harvesting/Reaction Center System.* J Am Chem Soc, 2014, 136, 16618

9:35 (10 min) - Jens Viefhaus: Molecular physics at Petra III

9:50 (10 min) - Benjamin Erk: Molecular physics at FLASH

10:05 (20 min) - Tim Steimle: Spectroscopy of Heavy Metal Containing Molecules

Abstract: Two possible areas for DESY/ASU collaboration involving heavy metal containing molecules will be presented.

a) Electric dipole moments: ^{181}TaN.

Searches for permanent electric dipole moments, EDMs, of nucleons, nuclei, atoms, and molecules are effective, low-energy, venues for testing the Standard Model (SM). Permanent EDMs of elementary particles are highly suppressed in the SM (electron: $\left|d_e^{SM}\right| < 10^{-38} e \cdot \mathrm{cm}$; proton and neutron: $\left|d_{n,p}^{SM}\right| < 10^{-32} e \cdot \mathrm{cm}$. 10^{-38} e·cm), whereas newer theories often predict orders of magnitude larger values. Significant efforts have been made to establish increasingly lower upper limits on the electron's electric dipole moment (eEDM), $|d_e|$, which is currently 8.7×10^{-29} $e \cdot \mathrm{cm}$ and was obtained using thorium oxide, ThO[1]. In the hadron sector, the *T*, *P*-odd magnetic quadrupole moment (MQM) of the nucleus is another source of an atomic or molecular EDM[2]. Recently it was found that the sensitivity to this *T*, *P*-odd effect could be very high in paramagnetic molecules containing deformed nuclei[3]. ^{181}TaN in its low-lying metastable $^3\Delta_1$ states is the most promising candidate for detection of a nuclear MQM induced EDM. Our recent spectroscopic studies of ^{181}TaN will be described.

b) Thorium and Uranium Chemistry as a Proxies for Transuranium chemistry

Approximately 11% of the world's electricity is derived from nuclear power but the long-term nuclear waste storage and amelioration of the existing waste are primary concerns. The 4% enriched uranium fuel used in a typical light water reactor (LWR) is converted to spent nuclear fuel (SNF) made up of 3% fission products and 1% transuranium (TRU) elements Np, Pu, Am and Cm . Pu is the main contributor to long term radiotoxicity. Currently Pu and U mixed oxides (MOX) are often removed from the SNF and reused as fuels. If the remaining TRU elements could be effectively extracted from the SNF the mandatory storage time of the remaining waste could be greatly shortened. Furthermore, it may then become possible to treat the extracted radiotoxic TRU elements waste via neutron fission (nuclear transmutation) to produce a less radiotoxic sample. Given the societal implications of solving problems associated with treating, transmuting, monitoring, and storage of SNF, there has been an intense effort to understand actinide chemistry. Due in part to experimental difficulties, computational modeling is of heightened relevance for garnering insight. Here I will summarize our spectroscopic studies of gas-phase depleted uranium and thorium containing molecules[4,5] . The determined fundamental properties (molecular frame dipole moments, hyperfine interactions, structure, etc.) are being used for assessing various computational methodologies, basis sets, and functionals being developed.

References

1. J. Baron, et al. Science (Washington, DC, U. S.) **343** (6168), 269-272 (2014).
2. B. M. Roberts, V. A. Dzuba and V. V. Flambaum, Annu. Rev. Nucl. Part. Sci. **65**, 63-86 (2015).
3. V. Flambaum, D. DeMille and M. G. Kozlov, Phys Rev Lett **113** (10), 103003 (2014).
4. Steimle, T., Kokkin, D. L., Muscarella, S. & Ma, T. *J. Phys. Chem. A* **119**, 9281, (2015).
5. Kokkin, D. L., Steimle, T. C. & DeMille, D.. *Phys. Rev. A: At., Mol., Opt. Phys.* **91**, 1 (2015).

10:30 (20 min) - Robin Santra: The CFEL-DESY Theory Group

10:55 (20 min) - Scott Sayres: Electronic Processes in Strong-field Ionization

Abstract: Strong-field ionization has become the workhorse of modern ultrafast spectroscopy, and also a powerful tool for determining the electronic structure of atoms, molecules, and clusters [1]. When synchronized to another laser pulse through the pump-probe technique, this attosecond process may be used to explore electron reconfiguration and also arrest the intermediates of ultrafast photochemical reactions. I will present our progress in exploring how the ultrafast dynamics of small, solvated acid clusters depend on the addition or subtraction of a single water molecule. These strong acid clusters serve as ideal systems for exploring non-Born Oppenheimer processes.
References: S. G. Sayres, M. W. Ross, A. W. Castleman Jr. Influence of clustering and molecular orbital shapes on the ionization enhancement in ammonia. Phys. Chem. Chem. Phys. **13**, 12231-12235 (2011).

11:20 (15 min) - Sebastian Trippel: Controlled Molecules for molecular-frame imaging

11:40 (15 min) - Melanie Schnell: Disentangling the building blocks of life

12:00 - Jochen Küpper & Tim Steimle: discussion and wrap up

Confirmed impulse talks (1 slide / 90sec) in discussions:

- Tim Laarmann: Molecules and Clusters in New Light
- Sang-Kil Son: XMOLECULE: ultrafast ionization and fragmentation dynamics by XFEL pulses
- Oliver Mücke: Ultrashort-pulse lasers and XUV sources for ultrafast molecular dynamics studies

Parallel Session B2: Biology with Free Electron Lasers and SFX method developments (CFEL Seminar Room I)

DESY: H. Chapman (co-chair), Anton Barty, …

ASU: P. Fromme (co-chair), John Spence, Wei Liu, Alexandra Ros, Brenda Hogue, Thomas White, …

CSSB: Matthias Wilmanns

Schedule:

1. Biology and macromolecules

09.00 Matthias Wilmanns (CSSB and structural biology on Bahrenfeld campus) – Visions on integrative structural biology
09.10 Brenda Hogue (ASU) – XFELS and Virus Biology
09.20 Lars Redecke (U of Luebeck/UHH/DESY) - in vivo crystallisation
09.30 Discussion of collaboration possibiities

2. X-ray methods

09.45 Alke Meents (CFEL) - Picosecond serial crystallography at PETRA III
09.55 Arwen Pearson (CFEL)
10.05 Wei Liu (ASU) - Femtosecond Crystallography of Membrane Proteins in LCP

Abstract: "The Center for Applied Structural Discovery (CASD) aims at establishing a structure-based drug design (SBDD) platform for G protein-coupled receptors (GPCRs) built upon our recent technical breakthrough combining lipidic cubic phase with serial femtosecond crystallography (LCP-SFX). SBDD has achieved great successes on soluble protein targets, including kinases and proteases, yet is much less productive on membrane proteins such as GPCRs, mainly due to the recalcitrance of the latter to form homogenous samples and generate sufficiently large crystals needed to collect high-resolution diffraction data at synchrotron beamlines. The LCP-SFX technique works effectively on microcrystals grown in LCP from only sub-milligram quantities of purified protein, and thus surmounts the obstacles associated with traditional synchrotron beamlines. By continuously delivering the fully hydrated GPCR microcrystals embedded in LCP, SFX at Linac Coherent Light Source (LCLS) enables the collection of hundreds of thousands high-resolutions diffraction data. This novel technique has proven successful in structural determination of several GPCRs. We will further optimize the LCP-SFX technology for structural determination on GPCRs, target several receptors/ligand co-crystal structures at atomic resolution, and establish an SFX-SBDD platform for GPCRs as well as many other membrane proteins."

10.15 Discussion of collaboration possibilities

10:30 Coffee Break

3. Sample delivery

10.45 Ken Beyerlein (CFEL) - Recent Sample Delivery Developments at CFEL
10.55 Alexandra Ros (ASU) - Microfluidics for Serial Femtosecond Crystallography and Beyond
11.05 Discussion of collaboration possibilities

4. Software and analysis methods

11.15 Anton Barty (CFEL analysis methods development)
11.25 Thomas White (CFEL) – Methods and tools for XFEL and serial crystallography data processing
11.35 Kartik Ayyer (CFEL analysis methods development)
11.45 Discussion of collaboration possibilities

12:15 Working Lunch for DESY/ASU Participants

12:00-13:00 Closed Meeting on DESY-ASU Collaboration Governance /Steering

- *Participants: Helmut Dosch, Edgar Weckert, Frank Lehner (DESY) - William Petuskey, Neal Woodbury, Roger Johnson (ASU) plus Micol Martinelli (via phone)*
- *Strategy and structure of cooperation, including:*
    - *Mobility, education/exchange students/postdocs, staff, sabbatical*
    - *Research rotation*
    - *Organizing a joint PhD program, Graduating from ASU?*
    - *…*
- *Joint appointments/hiring*
- *Research funding, linking with other funding frameworks, embedment in Helmholtz context*

13:00 Final Plenary (FLASH Seminar room)

- Reports from the parallel session chairs (addressing questions mentioned below)
- Discussions
- Conclusions, next steps

14:30 Tours of Facilities

Key Questions for the sessions to be addressed:

The workshop should promote joint DESY-ASU research activities with the goal to arrive at a more structured form of DESY-ASU cooperation. Convenors in their session are asked to address the following key questions and report back in the plenary:

- Where is the field today, what are the grand challenges/holy grail to be specifically targeted at?
- What is available (at DESY and ASU) and what is needed in terms of expertise, methods, instrumentations/facilities, infrastructures, access …
- What ideas exist for a joint pilot/demonstration experiment/project to quickly initiate (near-term)? What could be a grand flagship project of a DESY-ASU partnership (mid/long-term)?
- What other partners need to be involved? Also, how to embed this cooperation in a larger context, e.g. Helmholtz?
- What cooperation structures/frameworks/instruments would help to advance the partnership?
    - Bilateral mobility/exchange schemes, seed money, joint project funding?
    - Is there a perspective for a larger third party funded project application?
    - Is there an opportunity for a specific targeted joint (DESY-ASU) hiring on a professor level?

Useful Information DESY-ASU Workshop

Location:

The workshop will take place at the site of DESY (http://www.desy.de) located in the west of Hamburg. DESY has two entrances: a main entrance located at Notkestrasse and a side entrance at Luruper Chaussee. The main entrance is open all day and night. The side entrance is open for motorists from Monday until Friday, 06:00 to 19:00, and closed on weekends. It is open for pedestrians and cyclists at all times. The gate keepers at the DESY entrances will provide you with a map of the DESY campus. The DESY campus is signposted to point you to the right buildings.

Please check the following website to learn more about how to get to DESY from the airport or train station and also for a DESY campus map:

http://www.desy.de/about_desy/getting_there/hamburg/index_eng.html

Accommodation:

We have made the booking arrangements in the Hotel Mercure (in close proximity to the campus) on a self-payment basis. From the Mercure Hotel you can easily walk to DESY within 10 minutes. We offer a DESY shuttle from the Hotel Mercure to DESY on

- Wed, 27 April at 16:45 for the Welcome Reception from Mercure to DESY building 1
- Thu, 28 April at 08:30 from Mercure to FLASH Seminar room
- Fri, 29 April at 08:30 from Mercure to FLASH/CFEL 2016.

WLAN:

There will be WLAN available to the workshop participants. Please connect to **DESY-Guest** requiring you to fill out a Web form on our portal server and register your mobile device (e.g. notebook). For participants, whose home institutes are participating in the project **eduroam**, we offer also this wireless guest network connection. For registered user this is a quick and easy way to obtain a secure access to the Internet without any further registration.

Registration

The workshop registration is free. DESY covers reception, coffee breaks, lunch and the workshop dinner.

Sightseeing in Hamburg

With its flair and its maritime charms Hamburg counts amongst the most beautiful cities in Germany. The "Gateway to World" - as the seaport on the Elbe river is also frequently called - offers pure city life with unique shopping, culture but also nature experiences.

Information about sightseeing spots are available on the Hamburg Tourismus website (http://english.hamburg.de)

For questions please contact the local workshop organizer

- Frank Lehner, DESY, Phone: +49 40 8998 3612; E-mail: frank.lehner@desy.de
- Sabine Berger, DESY, Phone: +49 40 8998 5613; E-Mail: sabine.berger@desy.de
- Emergency Mobile: +49 1511 2225768 (Frank Lehner)

Campus Map