CUI NEWS





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RESEARCH

Dear reader!

Almost six years have gone by since our interdisciplinary research project got started. We have reached many goals, but in doing so we have also realized how exciting our research field is and how many fascinating new aspects are still evolving.

In this "best of" version of our German CUI News we are shining light in the truest sense of the word on molecular dynamics and the progress we have made in our research areas. It is an interplay between different partners, different scientific fields such as physics, chemistry and molecular biology, and between theory and experiment. Read what our colleague Ludwig Mathey thinks about the dialogue between theory and experiment, why Christian Bressler feels a little like Starship Enterprise, and why a dream comes true for Arwen Pearson.

Our research covers a wide field scientifically, but also with regard to social aspects. It is very important for us to support young researchers and provide them with the best opportunities. The interdisciplinary concept of our graduate school allows them to dive deeply into their own projects while at the same time they have the chance to meet with experts directly from their field or from other projects. As it turned out, it is most fruitful to let them develop their own schools and workshops.

Speaking of schools, our school laboratory "Light & Schools" has developed an extensive program over the past years. So we are extremely happy about the new building "HAUS DER LEHRE – LIGHT & SCHOOLS" for which the foundations were laid at the beginning of 2018. We want to build bridges between schools and the university, between research and teaching.

This includes the broader public. We are therefore rather proud of the success story of our exhibition "Arts & Science" which was shown for the first time in Hamburg's City Hall and which was visited by thousands of people.

Enjoy reading!

Prof. Dr. Klaus Sengstock Prof. Dr. Horst Weller Prof. Dr. R. J. Dwayne Miller **CUI** spokespersons



AREA A: CONTROL OF MATTER WITH LIGHT

LIGHT CAN DO SPECIAL THINGS

cientists doing research in Area A use the most modern sources of light to learn more about its effect on matter. In fact, the explored objects are quite different; these might be single atoms or simple molecules, but also complicatedly structured solid state materials. Moreover, the used light is very "colorful"; the wavelengths cover the THz range (approx. $300 \ \mu$ m), the visible range (~ $0.5 \ \mu$ m) and wavelengths down to hard X-ray radiation (0.0001 µm). This is one of the reasons why research in Area A is subdivided into four focuses. The shared vision, however, is the same: Once we understand on the guantum level how matter reacts to light, we will find ways to use light for systematically controlling and steering materials which build up our world and determine its behavior.

The negatively charged electrons found in all matter react especially sensitivly to the alternating electric field related to light. In Research Focus A.2, Professor Franz Kärtner (Universität Hamburg, DESY, MIT) and his colleagues have succeeded in generating THz light waves with a field strength of 300 million volts per meter (Huang 2016). For comparison: in a thundercloud, the value rarely exceeds 1 million V/m. These enormous fields have the potential to accelerate electrons to high velocities within very short distances. As was shown in subsequent work by the group in Focus A.1 (Putnam 2017), a very good source for electrons are nanoscopic structures which are arranged on surfaces in a regular pattern. With short laser pulses, and supported by electron oscillations

in the rhythm of the laser field (plasmons), the electrons are released from the surface as equally short charge pulses.

Light refraction as in a crystal

Moreover, electrons also determine the optical behavior of materials. In cooperation with Professor Christian Bressler (European XFEL) (Zalden 2016) it was observed that strong THz waves in liquids such as water, alcohols and oils induce the formation of double refraction. This means that a usually completely isotropic medium suddenly shows a differing refractive index in various directions, thus behaving like an anisotropic crystal during THz irradiation. Again – as is the case with many other of its properties - water exhibits odd characteristics and behaves anomalously compared to other liquids. In this context it is also remarkable, how nanoscopic particles - as they are produced and analyzed in CUI Research Area C - behave when they are dissolved in such a liquid. A theoretical study by the team of Professor Michael Thorwart (Universität Hamburg) describes how nanoparticles behave in a liquid bath when a strong alternating electric field acts on the bath (Grabert 2016).



Very distant lasers may be synchronized

With the use of X-ray beams, it is possible to experimentally investigate the dynamic behavior of molecules or particles in a liquid environment with a high spatial resolution and, with the short pulse duration of freeelectron lasers (FELs), with a high time resolution as well. However, short X-ray pulses are not sufficient - they must also be synchronized stably enough with the exciting (THz) pulse. Unfortunately, it has been shown that, at most FELs, the fluctuations of synchronization are significantly larger than the pulse duration. Scientists led by Professor Franz Kärtner were recently able to demonstrate (Xin 2017) that at large X-ray FEL's, it is possible to synchronize auxiliary lasers, which are separated from each other by several kilometers, with attosecond-scale precision.

A completely different approach has been proposed by Professor Robin Santra (Universität Hamburg, DESY) and Professor Tamar Seideman, who in 2013 was awarded the Mildred Dresselhaus Guest Professorship established by CUI. This theoretical work (Fung 2016), which resulted from their collaboration, deliberately accepts fluctuations and proves that, with a skillful analysis of the temporally "blurred" data, it is possible to bring to light the hidden dynamics of the observed process. This allowed the extraction of a periodicity of 15 femtoseconds from an old data set of measurements on molecular nitrogen with a statistical time uncertainty of 300 femtoseconds that could be allocated to a vibration of the molecule. It is obvious, of course, that the observation of freely floating molecules becomes easier when these are spatially oriented. In collaboration with the first winner of the Mildred Dresselhaus Guest Professorship, Professor Rosario González-Férez, Professor Jochen Küpper (Universität Hamburg, DESY) demonstrated (Kienitz 2016), how to align OCS molecules in space with the help of mixed static and dynamic electric fields.

(Continued on page 4)

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CONTINUED: LIGHT CAN DO SPECIAL THINGS

Barriers become permeable, transition temperature rises

Compared to molecules, the temporal evolution of states in atomic clouds is considerably slower when these are cooled down to temperatures approaching absolute zero. However, Focus A.3 reveals that the sudden ionization of parts of an ultracold quantum gas entails a distinctive dynamic development on the µs to ms time scale. The interaction of a thereby generated single ion with the remaining quantum gas could already be theoretically described to a great extent. As it was demonstrated by Professor Peter Schmelcher's group at Universität Hamburg (Schurer 2016), the dynamic behavior of a Bose-Einstein condensate (BEC) is strongly influenced by the spin of the ion embedded within. Thus, it is possible, for example, to "switch" the permeability of quantum-mechanical tunnel barriers.

Bose-Einstein condensates have even more fascinating properties. In Focus A.4, the team of Professor Henning Moritz gives these quantum gases a two-dimensional structure and – jointly with Professor Ludwig Mathey (both Universität Hamburg) - investigates their superfluid behavior (Singh 2016). In a liquid with this property, friction disappears completely. Many other material properties, such as the quantum Hall effect, depend on its topological state. A collaboration of Professor Andreas Hemmerich (Universität Hamburg) with this year's Mildred Dresselhaus prize winner, Professor Cristiane Morais Smith, presented scenarios (Xu 2016, Di Liberto 2016) to investigate topologically driven excitations

with bosonic atoms in optical lattices. One topology-defining property is the so-called "Berry curvature". This factor, postulated for a long time but difficult to measure in real solid materials, was observed and measured for the first time in a quantum simulator (Fläschner 2016) by the team led by Professor Klaus Sengstock (Universität Hamburg). In this case, an ultracold quantum gas in a hexagonal light grid mimics the atoms in a crystal lattice.

Superconductivity is usually expected in metals or ceramic materials. Scientists in Focus A.4 already

showed that, upon irradiation with strong light fields, it is possible to notably increase the transition temperature. Currently, Professor Andrea Cavalleri and his team from the Max-Planck-Institute for the Structure and Dynamics of Matter investigated a seemingly exotic material consisting of C6o fullerenes networked via potassium atoms (Mitrano 2016). By using THz pulses, an increase of the transition temperature by more than 80 Kelvin could be verified. At the same time, Dr. Tim Laarmann (DESY) and Professor Markus

Drescher (Universität Hamburg), who coordinates Research Area A, initiated another study on fullerenes (Usenko 2016). In many respects, the 60 carbon atoms of the fullerene already behave like a solid and can develop a large number of oscillation modes. It is now possible to experimentally explore and theoretically interpret the coupling of an electronic excitation at such lattice vibrations on the fs-scale. The results suggest that the energy of the large number of oscillation modes is ultimately transferred again to the electron system, namely to orbitals looking like those of a simple atom.



The illustration shows a bosonic Josephson junction controlled by a single ion: Depending on the spin state of the ion, the atoms will either tunnel through (left) or they are "self-trapped" (right)

ANALYSIS IN OUTER SPACE

Carrier rocket brings protein crystals to the ISS



n 19 February 2017 a carrier rocket was launched to the International Space Station (ISS). Samples from Profesor Christian Betzel's research group at Universität Hamburg were on board to be analyzed in the absence of gravity.

The experiment in the context of the CUI research was aimed at optimizing the growth of micro- and nanocrystals. "In the absence of gravity, there is no convection or sedimentation which means that protein crystals can grow better and are of higher quality, lacking defects, and more pure," Betzel explains. It is exactly this process, the researchers wanted to analyze in detail.

Crystals help to determine the three dimensional structure and function of biomolecules at atomic resolution. This is significantly important for researching the basic components of life and understanding illnesses.

The samples for the experiment on the ISS were prepared in December 2016 at NASA, USA. The researchers chemically modified certain proteins, thus contaminating the protein solutions, which were used for crystallization experiments on the ISS in accurately calculated concentration series. The scientists wanted to observe the process of contamination in space and compare it with experimental results on earth in order to understand how gravitation contributes to contaminations in crystals.

The ISS was equipped with a special microscope (LMM, Light Microscopy Module) the data of which were live video transmitted to a protected computer system in the working group's laboratory at the Institute for Biochemistry and Molecular Biology. Back on earth the crystals were further analyzed with synchrotron radiation at DESY and mass spectroscopy. The results from this research project contribute to the targeted production of protein crystals, which are also used at the European XFEL.

The project was also supported by the German national aeronautics and space agency (Deutsche Agentur für Luftund Raumfahrt, DLR).



Prizes and awards I.



Prof. Horst Weller, Head of the Institute of Physical Chemistry at Universität Hamburg, was invited to the renowned Matthiae Meal 2018 in the ballroom of Hamburg's City Hall and is to receive the "Colloid & Interface Science Award, sponsored by Solvay'

of the European Colloid and Interface Society (2018).

In recognition of his work on the SurePIRL project Prof. R. J. Dwayne Miller (MPSD) is to receive the 2018 European Physical Society (EPS) Prize for Laser Science and Applications. He was also named distinguished Alumnus by the University of Manitoba.



In 2017 Miller received an honorary doctorate from the University of Waterloo in Canada. He has also won the Centenary Prize 2016 of the Royal Society of Chemistry and has been invited to become a fellow. Furthermore, a joint research team of the MPSD and the University Medical Center Hamburg-Eppendorf (UKE) was awarded the Dr.-Karl-Robert-Brauns-Prize for ophthalmology 2016 for their research on laser eye surgery.



Prof. Peter Schmelcher, from the Center for Optical Ouantum Technologies of Universität Hamburg, has been elected by the American Physical Society into the executive committee of the Topical Group on Few-Body Systems and Multiparticle Dynamics (2018).

Prof. Andrea Cavalleri (MPSD) has been awarded the 2018 Frank Isakson Prize for Optical Effects in Solids by the American Physical Society and has been elected member of the European Academy of Sciences (EURASC). In 2017 he was elected a Fellow of



the Association for the Advancement of Science (AAAS). He has also been chosen as a member of the Academia Europaea – a non-governmental body which promotes research and scholarship across Europe. In addition, he has received the Dannie-Heineman-Prize 2015 from the Minna-James-Heineman-Foundation Hannover.



Prof. Henry Chapman (UHH, DESY) has been named honorary doctor at the Faculty of Science and Technology at Uppsala University in Sweden (2018). In addition, he was invited to the renowned Matthiae Meal 2016 in the ballroom of Hamburg's City Hall and

in 2017 he received the Roentgen Medal of the City of Remscheid. In addition, an international team of researchers including Chapman has been awarded a research grant by the Human Frontier Science Program to develop a novel method for imaging individual biomolecules with atomic resolution. The team will receive a total of US\$ 1.35 million over a period of three years (2017).

AREA B: GREAT PROGRESS IN CRYSTALLOGRAPHY REVOLUTIONIZES STRUCTURAL ANALYSIS

FROM THE LIFE OF BIOMOLECULES

ow can we understand complex systems? CUI scientists combine the investigation of structure and of dynamics on all time and length scales. One focus is on the analysis of biochemical processes on the molecular and atomic level in diffraction experiments with the new ultrafast electrons and X-ray beams. In the Research Area "Atomically Resolved Structural Dynamics", coordinated by Professor Henry Chapman (Universität Hamburg, DESY), small and large systems and structure-function correlations are investigated and at the same time new methods are developed and applied. The goal is to get a broader understanding, thus allowing to give answers to the urgent questions of biological and medical research.

The starting point includes already well understood model systems, e.g. the Pt(dmit)2 compound studied in the group of Professor Dwayne Miller using femtosecondduration electron pulses. In terms of its size and complexity, it corresponds to a small protein and forms a crystal with a unit cell of four nanometers. In this case, the dynamics which stabilize the charge separation were investigated. This produced spectacular films of atomic processes, as it is possible to see the dimensionality reduction during the structural transition with the naked eye. Thus, the investigation allowed the team to take a look at what is really essential in the process of a chemical reaction (Ishikawa 2015).

Following on the longstanding developments in the field of diffraction from pulsed electron sources and synchrotron radiation, the high brilliance and the extremely short pulses of free-electron lasers also offer completely new possibilities for time-resolved protein crystallography (Miller 2014). In a proof-of-principle investigation, CUI scientists demonstrated that serial femtosecond crystallography using micrometer-sized crystals provides very precise time-resolved structural images. Thus, it was possible to determine the structures of the so-called photoactive yellow protein at several points of time within the photocycle. As the very small crystals can be uniformly excited, much better results can be obtained than by means of synchrotron Laue diffraction (Tenboer 2014; Pande 2016). Although steadily improving (Oberthuer 2017), a potential disadvantage of the method is the high demand for samples. This can be solved by using photo-crystallographic chips which are rasterized through the pulsed beam (Mueller 2015). When using the new technology with myoglobin, the data indicate that collective coordinates on fast time scales shape the dynamics. This is in line with the collective modes model, proposed by Miller already in the time between 1989 and 1991, to understand structure-function relationships.

Structure-function relationships are generally one of the research focuses at CUI. One example is the investigation of the structure of a RNA oligonucleotide, which leads to a category of novel drugs. These show a promising efficacy in phase II clinical trials on patients with diabetic kidney disease (Oberthür 2015). Other studies investigate possibilities of where drugs can be targeted to fight malaria



Illustration of the new macromolecular crystallography concept for disordered crystals

(Perbandt 2015) and how the immune response to Yersinia infections takes place in cells (Berneking 2016).

Femtosecond pulses at free-electron lasers also offer a number of advantages to determine the structure itself, as the pulse stops before the sample is destroyed. This allows the exploitation of data from crystals smaller than 100 nanometers (Gati 2017). Samples can be examined at physiological temperatures and must no longer be cryogenically cooled. The methodical improvements have the potential to revolutionize structural biology because they enable analyses of structures which so far were not accessible, e.g. the rhodopsin-arrestin complex (Kang 2015).This structure shows how signal transduction is regulated in cells and why a certain category of drugs has lesser side effects.

When non-perfect crystal lattices are used, Bragg peaks can only be measured to a limited scattering angle, which limits the resolution of the structure that can be recovered, even with the full brilliance of a free-electron laser. However, the disorder in such crystals produces a diffuse background within the diffraction patterns which had not previously been fully interpreted or utilized in determining structures. In case of random deviations from the ideal lattice positions, this diffraction can be interpreted as the incoherent sum of single-molecule diffraction of individual complexes. This simple concept (see illustration 2) leads to a new paradigm in crystallography –ordered crystals are no longer the most suitable for the best analysis, preferable are imperfect crystals. This new analysis method makes possible not only higher resolutions but at the same time

offers a more robust method for structure determination (Ayyer 2016).

The new possibilities offered by the ultra-brilliant electron and X-ray radiation sources change protein crystallography in other areas as well. Some organisms are capable of producing nanocrystals by natural means, for example yeast cells. Even using whole cells, it was possible to obtain diffraction data of excellent quality from these nanocrystals at room temperature, without the necessity for complex protein purification. This opens up promising possibilities to use cells as a kind of crystallization factory (Jakobi 2016). Moreover, new methods were developed which allow the characterization of protein nanocrystals. Already during their growth, it can be seen whether these are nanocrystals or only non-crystalline protein aggregates (Schubert 2015, CUI News July 2014).

A basic prerequisite for any time-resolved measurement is that synchronous reactions must take place in all molecules of the sample. If this is not the case, the details of the process appear in a blurred way. Thus, most time-resolved measurements were so far carried out using naturally occurring photo-induced systems; however, these represent only a fraction of the systems to be submitted to dynamics investigations. Since 2015, CUI groups have been working to make additional systems amenable to a time-resolved investigation. For very fast processes, such as enzyme catalysis on a time scale, photochemical reagents are being developed which allow the triggering of biochemical reactions using very short laser pulses. For slower processes, such as the assembly of virus capsids or the

Prizes and awards II.



postdoctoral position.

assembly of 2016.

Dr. Roman Mankowsky (MPSD) has been awarded the Reimar-Lüst-Prize by the Max-Planck-Society, including a two-year

Prof. Günter Huber

(UHH) was elected

as an external

member of the

Russian Acade-

my of Sciences

Dr. Briony Yorke

(UHH) gave the

Parkin lecture at

2017 of the British

Crystallographic

Association (BCA),

which addressed the translation

and was thereby honored for her

of crystallography into music,

during the general

four-year Sir Henry Wellcome Postdoctoral Fellowship (2016).

Prof. Dr. Alexander Lichtenstein (UHH) has been awarded the title "John von Neumann **Excellence Project**" of the John von Neumann Institute for Computing (2016).

Prof. Arwen Pearson (UHH) has given the Lonsdale Lecture at the Spring Meeting 2016 of the British Crystallographic Association (BCA). A joint research project led by Pearson was also granted € 2 million by the Federal Ministry of Research (BMBF). The project "Hadamard crystallography as a method for time-resolved





transport of ligands across cell membranes, microfluidic devices are being developed. These mix reagents in a tiny reaction chamber before making them accessible via a jet system for structure elucidation (work groups of Huse, Tidow, Trebbin, Pearson).

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outstanding engagement to public outreach. She has also obtained a

investigation of the structural dynamics of biomolecules" includes the groups of Prof. Nils Huse (UHH), Dr. Thomas Schneider (EMBL Hamburg), Prof. Henry Chapman (DESY, UHH), Prof. Christian Betzel (UHH) and Prof. Martin Trebbin (UHH).



Dr. Philipp Wessels (UHH) won a **German Student** Award of the Körber foundation (second prize, 2016). He has also

been invited to the 2016 Lindau Meeting of Nobel Laureates.



Thanks to the support of CUI, Dr. Florian Schulz (UHH) was able to raise funds worth € 330,000 from the DFG to support his

research field "Flexible synthesis of stable nanoparticles of gold" over three years (2016).

RESEARCH



AREA C: COHERENT X-RAY LIGHT DECODES DYNAMICS ON THE NANOSCALE

NEW METHODS ALLOW DEEP INSIGHTS

he study of ultrafast ordering phenomena is of crucial importance for both, the understanding of materials and the development of "tools" for nanoscience. In Research Area C "Dynamics in Nanostructures", coordinated by Professor Gerhard Grübel (DESY), scientists work on getting a precise understanding of the dynamics of order formation on the nanoscale. For this purpose, three research foci were identified, each using new sample environments, new measuring methods and state-of-art X-ray light sources.

Scientists at Research Area C.1, headed by Professor Gerhard Grübel, investigate the structure and dynamics of liquids and glasses in scattering experiments at modern X-ray sources. In order to discover even the smallest transient ordered states, the researchers use the highly intensive and ultra-short X-ray pulses of free-electron lasers (FELs) in the hard X-ray range, for example the Linac Coherent Light Source (LCLS) in the US, the SPring-8 Angstrom Compact free-electron Laser (SACLA) in Japan and the European XFEL in Hamburg, for the first time facilitate investigations of the dynamics of liquids over 18 orders of magnitude - from femtoseconds, that is one millionth of a billionth of a second, up to several 1000 seconds. Moreover, thanks to the high coherence of FEL X-ray pulses, it is possible for the first time to study the sample dynamics on length scales in the nanometer range. The disadvantage: unlike storage-ring experiments, as for example are carried out at DESY's PETRA III, the natural fluctuations of FEL X-ray radiation and the ultra-discrete time structure of FEL facilities may also aggravate such experiments. Particularly when using established methods, such as X-ray Photon Correlation Spectroscopy (XPCS) to measure fast sample dynamics, it is necessary to exactly characterize the source (Lehmkühler 2014). At storage rings, XPCS routinely enables dynamics experiments in the range of milliseconds up to several 1000 seconds. The foci in Research Area C.1 include investigations on diffusion and phase and glass transitions in soft matter (Conrad 2015) and

descriptions of local order (Schroer 2014, 2015; Lehmkühler 2014, 2016, 2018) by means of X-ray cross correlation analysis (XCCA).

In XPCS experiments at FEL's, scattering signals (speckle patterns) of at least two ultra-fast, but different X-ray pulses are compared (see illustration at top). In the experiments at SACLA and at LCLS, CUI scientists could demonstrate that conventional XPCS experiments with several 100 sequential pulses – with pulse intervals between 8.3 and 50 milliseconds - are possible, regardless of natural pulse-to-pulse fluctuations at FEL's (Carnis 2014; Lehmkühler 2015). By choosing established reference samples, they were able to investigate the properties of individual pulses with particular focus on XPCS applications. The results show that the European XFEL will offer the possibility to achieve faster time scales in conventional XPCS experiments to less than 1 microsecond by using the pulse intervals from 222 nanoseconds. The use of pulse split and delay optics allow additional improvement of the time resolution. In this case, individual X-ray pulses are split into two pulses, with one of them being delayed by up to several nanoseconds. First experiments were already carried out with prototype samples at LCLS and SACLA, and the possibility of the concept was demonstrated (Roseker 2018). In future, CUI scientists will routinely carry out ultra-fast-XPCS experiments to investigate the structure and dynamics of complex liquids. Of particular importance are, for example, the detection of transient pre-structures in the vicinity of phase transitions or the elucidation of water anomalies with XPCS and XCCA at supercooled water droplets (Steinke 2016; Perakis 2017, 2018).

Research Area C.2 (Professor Horst Weller and Professor Alf Mews, Universität Hamburg) investigates among others nucleation and growth of nanoparticles. One example is the nucleation of CdSe particles in time-resolved X-ray scattering experiments. Here, at a synchrotron radiation source, the

scientists observe the growth reactions in situ at different temperatures. For this purpose, collaborations of several CUI groups created different sample environments, particularly so-called microjets, which can inject micrometer-thick liquid jets into a specific environment, and various microfluidic channel systems with the sample liquid being pumped through thin channels. Due to the constant sample flow, it is possible to measure the development of the sample over time at different positions along the channel and thereby investigate the processes of time-resolved nucleation, growth and ion exchange (Bothe 2015, Lauth 2016). A modification of this sample environment is constituted by mixing channels, with two or more reaction partners being mixed inside the channels, to trace the following reaction over time. In the future, CUI scientists also plan to investigate the fluctuations of such processes, for example by using XPCS at FEL-radiation sources.

Coherent X-ray light from FEL and synchrotron radiation sources is also outstandingly suitable to image nanoscopic structures. With the newly developed X-ray holographic microscopy (XHM), scientists of Area C.3 investigate magnetic nanodots (Professor Hans-Peter Oepen, Universität Hamburg). The analysis of magnetic nanostructures and their interaction is of great importance, as these structures are candidates for digital data storage and processing. The illustration to the right shows an example in which CUI researchers examined nanodots of 60 nanometers in size. The study of magnetization processes of nanostructured materials is a forefront topic in the modern magnetism research, particularly after the proposal was made to use pulses in the terahertz range (Bocklage 2016), which allow the quantitative study of such processes (Professor Ralf Röhlsberger, Dr. Giodo Meier).

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a) Sample of differently aligned magnetic bits on an X-ray permeable film. Red and blue arrows symbolize the vertical component of magnetization. The sample is irradiated from above with circularly polarized X-ray radiation.

b) Scanning electron microscope image of the lithographically produced structure.

c) Holography taken with a camera behind the structure. The difference of left and right hand circularly polarized light shows a magnetic diffraction image of the structure.

d) Reconstructed difference hologram reproducing the magnetic status of the individual bits. Red circles mark three bits with a magnetization direction opposed to the others.

Prizes and awards III.



The Optical Society of America (OSA) has elected Prof. Franz Kärtner (UHH, DESY, MIT) as a Director at Large (2016-2018).



Dr. Xinxin Cheng (MPSD) has received a research fellowship for Postdocs from the Alexander von Humboldt Foundation (starting 2016).



Dr. Cornelius Gati (former CUI PhD student) has been awarded a Long-Term Fellowship for Postdocs by the International Human Frontier Science Program Organization (2015).



Dr. Melanie Schnell (DESY, Universität Kiel) was honored with the Academic Prize of Chemistry 2015 by the Göttingen Academy of Sciences and Humanities.

RESEARCH / APPLICATION

The illustrated FXE instrument enables the examination of chronological processes in liquids, solid state materials, and gases

VENTURING BRAVELY INTO THE UNKNOWN

Year ago, an important part of the European XFEL X-ray laser became operational. The so-called injector, the 45 meter-long forward part of the superconducting particle accelerator, brought the first electrons almost up to the speed of light. This was a crucial milestone on the journey to the completion of the installation which will offer completely new research opportunities for natural scientists and industrial users. On 1 September 2017 user operation started with one beamline and two experiment stations. CUI member Professor Christian Bressler is a leading scientist at the European XFEL and has been developing tools for femtosecond X-ray experiments for the past seven years.

Prof. Bressler, what does the construction of the European XFEL mean for you and for your scientific research?

I find the scientific perspectives which we are opening up hugely exciting. It feels a little like Starship Enterprise: we will see what no one else has ever seen before. The six different instruments at the European XFEL present fantastic research possibilities; the scientific instrument FXE, for example, allows scientists to observe a chemical reaction in all its electronic and structural detail and to measure it down to the atomic level (see box to the right).

What does fundamental science require from a large scientific instrument like the European XFEL in order to succeed?

First and foremost: the highest scientific standards. The current cutting edge of research represents the yardstick for this. A lot of scientific inspiration is needed in order to design such an innovative instrument, which is nurtured by the broad range of ideas from the scientific community. My team has the required inspiration and deep insight, but we have to constantly work on sustaining their creativity. Here, freedom of scientific research is one key ingredient next to an open exchange of ideas. A good cooperation with external experts – also because scientists from extremely different disciplines will work with our instrumentation – is needed for the continued improvement of our research opportunities.

But one also must want to bravely go where no one has been before, which includes trying out ideas for which we cannot foresee the outcome. That is important, because you basically enter a new continent with a machine like this, whose brilliance exceeds that of conventional sources by a factor of a billion, and it usually takes time until the possibilities become clearer. This is where the integrity of science comes into play, because the temptation is great to quickly



ad personam

Prof. Dr. Christian Bressler obtained his doctorate in 1995 at the FU Berlin and came to the University of Lausanne following a postdoctoral placement at SRI International in California. During his promotion professorship, he relocated to ETH Lausanne and developed time-resolved X-ray absorption spectroscopy tools at synchrotron light sources with synchronized lasers. Since he became a leading scientist at European XFEL, he is working on the development of simultaneously deployable complementary X-ray methods at free-electron lasers and synchrotron radiation sources. At the same time, his working group has built an advanced scientific instrument at the European XFEL, which was made available to the international scientific community in 2017.

publish premature results. In a healthy scientific atmosphere, this temptation does not exist. Hamburg certainly offers such an atmosphere and I also seek to safeguard this through my teaching for future generations.

How does the construction of this instrument affect the work in your group?

First of all, our task at European XFEL is the consolidation of the scientific instrument FXE and for this I meanwhile have a team of 7 experienced scientists and 3 engineers. We are about to recruit two further scientists, in order to also facilitate the day-to-day operation with external users. At the same time, we continuously need to work at the level of the latest research in order to constantly update the possibilities at our instrument. This is also paramount in order to help my scientific group members develop their own scientific careers. Such research work can only be done with third-party funding, which frees up dearly needed resources for fundamental research. Thanks to CUI, the Collaborative Research Center (SFB) 925 and the European project EUCALL, my group has grown to 15 members. That is very nice but adds responsibilities which I take very seriously. For example, it is extremely important to shield the (currently) four doctoral students from the daily pressure surrounding the instrument. On the other hand, their presence at European XFEL gives them a first-hand deep view of the state-of-theart FEL instrumentation, which will also come in handy for their next steps following their PhD studies. Overall, we need to communicate extensively within the group, since our scientific fields covered are meanwhile quite broad and the instrumentation including novel detectors is at the edge of the technical development.

What drives you in all this?

My immediate motivation comes from an immense curiosity which has always been part of me. In my "former life", I was rather a particle physicist and did precise measurements of energy levels and natural constants. After that I landed in molecular physics with X-rays and structural analysis. When I look back, I think of my chemistry teacher at grammar school, who said that no one had ever really seen an atom. Today we do not just see the atoms but we observe their motions in real time and the measured data has become incredibly precise. That is extremely exciting and it makes me want to jump for joy. After all those years of trying to improve our measurement methods we can finally concentrate on the use of our developed X-ray methods to study things we have not been able to investigate before due to the low x-ray flux available. We only just started to operate our new scientific instrument and will soon carry out experiments which we considered impossible just a few years ago.

Your wish for the future?

We have to improve the theory. That is very important in preparation for the use of XFEL X-ray light. Currently we measure many new things and a stronger connection to theory could help us understand what is going on there. For example, I would like to tackle the area of so-called "Solvation Dynamics". If we manage to describe not just the reacting molecule but also its surrounding water molecules which are also involved in the reaction process, or possibly even to picture them in real time, it would be pioneering work. No one has managed to do that so far.

Thank you very much for the conversation.



European XFEL: light pulses of the highest brilliance and speed

Midway between the research campus Hamburg-Bahrenfeld and the town of Schenefeld, one of Europe's most ambitious research projects has been finished and started operation. The X-ray laser European XFEL will produce 27,000 light pulses per second, whose brightness is a billion times higher than that of the most intense conventional X-ray sources. Teams of scientists from all over the world will come to the European XFEL to study structures on the nano scale, ultrafast processes and extreme states of matter; they will generate three-dimensional images of viruses and proteins and film chemical reactions. They will have two soft and four hard X-ray instruments at their disposal:

- SPB / SFX Single Particle, Bio-imaging and Nano-crystallography: structural determination of single particles (atoms, clusters, bio-molecules, viruses, cells)
- FXE Femtosecond X-ray Experiments: examination of chronological processes in liquids, solid state materials, and gases
- MID Materials Imaging & Dynamics: structural determination of nanosystems and examination of nanoscale processes
- HED High Energy Density Science: examination of materials in extreme states
- SQS Small Quantum Systems: examination of atoms, ions, clusters in intensive light fields
- SCS Spectroscopy & Coherent Scattering: examination of the structure and dynamics of biological and nanosystems with soft X-rays

The facility was constructed and is being operated by European XFEL GmbH, an independent, non-profit body which cooperates closely with its largest shareholder, the research institution DESY, and other scientific institutions across Europe.

The construction and start-up costs of around 1.25 billion Euro (at 2005 rates) are being borne by Germany (57%), Russia (26%) as well as Denmark, France, Italy, Poland, Sweden, Switzerland, Slovakia, Spain and Hungary, and just recently: the United Kingdom (1-3% each).



The 3.4 km long European XFEL generates extremely intense X-ray flashes to be used by researchers from all over the world. The flashes are produced in underground tunnels and will allow scientists to map atomic details of viruses, film chemical reactions, and study the processes in the interior of planets

RESEARCH / APPLICATION

HARBOR: New CUI building will fill a gap and optimize excellent research infrastructure

MOVING TOWARDS A SCIENTIFICALLY ACCURATE MODEL OF LIVING CELLS



The new building will house a globally leading center for inter-disciplinary research in the areas of biophysics, bioorganic chemistry and structural biology

or Professor Arwen Pearson, a dream has come true: Last December saw the ground-breaking ceremony for the "Hamburg Advanced Research Centre for Bioorganic Chemistry", HARBOR for short, a project which has developed out of the CUI Excellence Cluster. "This will close the gap between the excellent physics and excellent life science research which is already present on the Bahrenfeld Campus," says the researcher in time-resolved structural biology.

In 2016, the Joint Science Conference of the Federal Government and its individual states adopted the recommendation of the Science Council and added the project to its funding program for 2017. The Federal Government and the City of Hamburg are contributing € 33 million to the building, the interior fitting-out and the large instruments. Pearson: "We now have the chance to set up a globally leading center for the study of the time-dependent properties of biological molecular machines." HARBOR establishes an inter-disciplinary center for nanophysics, chemistry and structural biology on the Bahrenfeld Campus.

Since Pearson commenced her research as CUI professor at Universität Hamburg in May 2014, she and her future HARBOR colleagues (see box) as well as CUI's scientific coordinator, Dr. Hans Behringer, have striven to create the perfect infrastructure for biophysics and bio-organic chemistry.

"With HARBOR, we have all the jigsaw pieces on one campus: brilliant light sources and beamlines, highly trained people and the appropriate laboratory infrastructure," delights the scientist, who spent many years working in England and the USA and now sets a new milestone as HARBOR's project leader. The aim: to create state-of-the-art premises and the necessary expertise in bio-(in)organic chemistry, photochemistry, physical biochemistry and computer-backed

modelling and simulation. This will enable the scientists to will develop light-based methods for the targeted triggering and control of processes in biological macromolecules in order to make these processes visible for study.

To explain: in order to generate a clear picture, the reactions in time-resolved experiments need to be triggered in such a way that all molecules to be examined react at the same time. In fast experiments, less than one millisecond, this can really only be practically achieved with light. Yet by their nature, only very few biological macromolecules react to light. Pearson: "This challenge of reaction initiation has meant the majority of interesting molecular biological systems were almost impossible to study using fast time-resolved structural experiments." HARBOR will pick up this challenge and develop the needed photochemical "tools", as well as provide facilities to help researchers characterize their systems and determine the optimal experimental set-up to address their scientific question.

In addition to the state-of-the-art modern facilities, HAR-BOR will also offer room for new and visiting research groups. "With a critical mass of bright people bringing together exciting scientific questions with cutting edge methods development, particularly regarding the theory, we will really be able to make progress," enthuses Pearson. CUI professor Gabriel Bester will be responsible for the theory section and supports Pearson as deputy project leader.

With nearly 3,000 square meters of floor space, the new building offers accommodation for around 130 people. Some 120 scientists will carry out their research in working groups focused on Spectroscopy and Imaging, Structural Molecular Biology, Synthetic Organic Chemistry and Theory. The following focal points have been defined:

- The time-resolved study of biomolecular systems requires universally deployable triggers which can initiate biological processes at a defined point in time. One major goal of the research is therefore the development and application of non-system specific photocages.
- The modelling of biomolecular processes with atomic resolution and high time-resolution is an ongoing challenge for numeric simulations. HARBOR research groups will therefore work on the development of numeric tools, to study the molecular dynamics of biological systems in experiments and computer simulations.
- · Initially the structural biology research working group wil focus on two key questions in biochemistry: How membrane proteins pass on signals and molecules across the cellular membrane and how protein dynamics regulate enzyme function.

"In the end, we would like to see a scientifically accurate, dynamic model of a living cell - but that will take decades,' says Pearson. This would make the vision of the molecular movie, which CUI has pursued in physics and chemistry so far, a reality in molecular biology as well. Pearson: "Then we will be able to answer fundamental questions about life and death, but also how we can make "green" chemistry a reality."

HARBOR will work closely with the research institutions on site as well as the national and international users of the facilities. Long before the building is handed over, which is set to happen in the middle of 2020, the

Teams, rooms, laboratories

The HARBOR research project has sprung directly from CUI's research. It is divided into four thematic focus points under the leadership of CUI scientists:



Prof. Arwen Pearson (Institute for Nanotechnology and Solid State Physics (INF), Universität Hamburg) is the project leader of HARBOR and responsible for the structural molecular biology working group.



Prof. Nils Huse (INF, Universität Hamburg) leads the spectroscopy / imaging working group.

The other groups in the building are led by Professor Henning Tidow (Institute for Biochemistry and Molecular Biology, Universität Hamburg) as well as Professor Alf Mews and Professor Horst Weller (Institute for Physical Chemistry, Universität Hamburg).

The offices and conference rooms of the scientists are distributed over three floors; 1,300 square meters of laboratory space are available on the ground floor and the first floor.

The following equipment will be available in the facility: super-resolution microscopy, X-ray crystallography, NMR, high-resolution mass spectrometry, flash photolysis and time-resolved spectroscopy as well as a computing cluster for molecular simulations.

The building is being erected directly next to the Center for Hybrid Nanostructures (CHYN) by Sprinkenhof GmbH based on drawings by the architects Nickl & Partner.





Ground-breaking ceremony: Hamburg's scientific senator Katharina Fegebank (2. from left), Dr. Martin Hecht, Head of Administration of Universität Hamburg (left), Prof. Dr. Arwen Pearson, scientific head of HARBOR, and Martin Görge, CEO of Sprinkenhof GmbH, reached for the shovels

fulfilment of the vision is underway. At CUI, the dynamic measurements have already started and a strong community across the campus involving research teams from UHH, EMBL, MPSD, EU-XFEL and DESY has already formed. "The strength of CUI lies in the fact that we could break down the frontiers between the disciplines. There is so much that we scientists can learn from each other and you do not need to re-invent the wheel each time," says Pearson. In fact, the interest of other groups has been sparked and structural biology, too, is increasingly visible at Universität Hamburg. Pearson: "It is already working."



Prof. Gabriel Bester (Institute for Physical Chemistry, Universität Hamburg) is the deputy HARBOR project leader, and leads the theory working group.



Prof. Chris Meier (Institute for Organic Chemistry, Universität Hamburg) is responsible for the Synthetic Organic Chemistry working group.

RESEARCH

THEORY AND EXPERIMENT

THE DYNAMICS **RAISES A NEW CLASS OF QUESTIONS**

he fundamental science at the excellence cluster CUI is an interplay on the most divergent levels. Here, colleagues from a wide range of national and international institutions cooperate; they research at the intersections of physics, chemistry, biology and medicine - with large scientific instruments, in laboratories and at computers. We spoke to Professor Ludwig Mathey from the Center for Optical Quantum Technologies at Universität Hamburg about one of the pillars of this system: the connection between theory and experiment in physics.

Professor Mathey, what is the task of theoretical physics?

Theoretical physics can be divided into two parts: on the one hand, it is about understanding an existing experiment that is the explanation of what has been observed. On the other, theoreticians generate suggestions for those in charge of the experiment as to what else could be measured - and in this way they prepare entirely new research directions.

Which role does mathematics play in this?

Mathematics is the tool kit. In the end, theory is a mathematical description. But while "real" mathematics is motivated by reality and leads to an abstract construct, physics is always a dialogue between the theory and the experiment.

What does this dialogue between the theory and the experiment look like?

The theory works with approximations and different methods, but always requires the feedback of the experiment. This is a very fruitful interplay. Because the other way around, the experimenters come to us with a measurement curve and ask how this may have happened. Then we gain a fresh impetus to think in a new direction, to develop new ideas. High-temperature superconductivity is a good example for this interaction. In the '90s, the models for existing materials had been calculated and the theoretical know-how trickled away, even though open questions remained. That stagnation came to an end, though, when Andrea Cavalleri experimented with new materials at the Max Planck Institute and gained new insights into these materials (see box for example). This has led to a tremendous revival. That is why the interplay between theory and experiment is extremely important and in the end the core of physical research.

Where are the boundaries of theoretical physics?

Physics is fundamentally limitless, but is - as demonstrated in the example I mentioned – limited in practice: through resources, through creativity or through materials. I am sometimes amazed, when it is said on television, for example, that we allegedly understand everything. Even independently of experiments there are many open questions and a list of challenges. The core subject of CUI, for example, the study of the dynamics of atoms, molecules and



The many phenomena of magnetism are of the greatest interest to fundamental and applied scientists. In a joint study, the groups of Mathey and Sengstock (Universität Hamburg) examined the formation of magnetic order in cold atoms. Red and blue triangles in this computer simulation represent different magnetic states which build domains of different size and form

solid state matter, raises a new class of questions. While light is being used in many parts of existing physics to measure a phenomenon that is occurring by itself, we now ask the question how superconductors, for example, can be influenced with the aid of light. So it is about the dynamical control of solid matter or atoms or chemical reactions through light. A lot of things are still unresolved here.

When is theory successful?

Generally we speak of a success when we understand a phenomenon. A theory has succeeded when an experiment is accurately predicted or accurately interpreted and fits into the complete physical framework. But sometimes calculations go wrong because the model or the approximation is flawed. I have often thought that one should start a journal of unsuccessful projects, because those projects can often lead to something that is right. It definitely has an intellectual value when one understands why something did not work out. An almost ideal example is a research result from Henry Chapman's group, which has been working on the blurring caused when working

with "disordered" crystals (see box). The exploration of a mistake or assumed mistakes leads to new insights.

Why are you doing all this? What is the societal mission?

Good fundamental science has a high social value in my eyes. It leads to applied science, to new technologies, to medical uses, to name but a few. The laser is a very good example of this. Its invention was regarded as a gimmick, a curiosity. Today, it is found everywhere: in cars, in medical technology, in almost all areas of everyday life and it is one of the most important technologies of the 20th century. But without fundamental physical science the laser would never have been invented.

The other societal mission is the training of young people. I always see a pronounced maturing process amongst our postgraduates. We pass on to them how you work in science – how to think analytically, set priorities and manage one's time. Those are all skills which are needed in science, but which can easily be transferred to other economic or industrial projects.

Thank you very much for the conversation.

Development of new materials

A study led by scientists from the Max Planck Institute for the Structure and Dynamics of Matter shows that superconductivity and charge density waves can coexist in connections of the rarely studied family of bismuthates. This observation opens new perspectives for a deeper understanding of the phenomenon of high-temperature superconductivity, a topic which has dominated research in solid state physics for more than 30 years. The present experiment, which the researchers around Professor Andrea Cavalleri and Dr. Daniele Nicoletti describe in PNAS, is a further example of how light can be used for the study, control and manipulation of materials. In the longer term, the aim of this field of research is to design a type of recipe for the development of new materials in order to reach new functionalities at increasingly high temperatures.

D. Nicoletti et al: Anomalous relaxation kinetics and charge density wave correlations in underdoped BaPb_{1-x}Bi_xO₂, PNAS 114, 9020-9025 (2017)

The solution lies in the disorder

A group of scientists around Professor Henry Chapman (Universität Hamburg, DESY) worked on the "background disturbance" of crystallographic scatter images, which occurs during work with "disordered" crystals. In the process, the group discovered that under certain circumstances this "background disturbance" contains the complete continuous scatter image of the single molecules in the crystal. This realization led to a paradigm shift in crystallography: the best ordered crystals are no longer those best suited to analysis in the new process. Those best suited are the slightly disordered crystals.

Ayyer K. et al: Macromolecular diffractive imaging using imperfect crystals, Nature 530, 202-206 (2016)





FOR LUDWIG MATHEY THERE ARE NOT MANY PLACES WHICH WOULD BE A BETTER THEMATIC MATCH

udwig Mathey has been Professor for Theoretical Physics at the Universität Hamburg since 2011 and leads the group Ultracold Atoms and Solid State Systems. As of 1 April 2017 he has accepted the call for a CUI theory professorship (W2). The chat with him about his career begins with a misunderstanding. How did he, a Professor of Physics, come to be a Doctor of Philosophy? Philosophy would interest him, yes, but the 'Doctor of Philosophy (Ph.D.), Physics is simply the American label of his doctor title in physics, says the scientist.

Mathey completed his doctorate between 2002 and 2007 at Harvard University in Cambridge, USA. He worked in a delocalized fashion, with different colleagues and not one single supervisor – a rather unusual situation compared to Germany. It meant that he had to kick off every project himself and was forced early on to become independent. "In the end I was very glad about the chance to mature during this process." Harvard, he says, is one of the global science centers and the exciting time there has changed him. "You realize, if I do not show some initiative, it will not work out," stresses the physicist.

In 2007, as a postdoc, Mathey went to the Joint Quantum Institute, which is run by the University of Maryland and the National Institute for Standards and Technology (NIST). 3,000 people work there on topics ranging from industrial use to fundamental scientific research. Mathey had already specialized on cold atoms and benefited from his very active environment - he worked, for example, with the Nobel Laureate in Physics Bill Phillips.

After three-and-a-half years as a postdoc, Mathey applied in the USA and in Europe: "The offer in Hamburg was the most attractive at the time. In 2011 there were three experimental groups for cold atoms, that is unusual. That was a near perfect match for me, because I was very much looking forward to the collaboration with them." In addition, there were the many other colleagues with whom joint activities have developed over time. And one felt that Professor Klaus Sengstock was trying to establish something with the Center for Optical Quantum Technologies. "That made an impression with me and the colleagues in atomic physics," Mathey says. After all he knew Professor Henning Moritz, one of the experiment leaders, from Heidelberg. For the scientist, who had grown up in Hamburg, it worked out well.

THINK TANK FOR THE FUTURE

Imost 6 years ago CUI's Graduate School accepted the first doctoral candidates. In an interview with CUI News Professor Peter Schmelcher, director of the Graduate School, describes the development of the school and sketches out ideas for the future.

Prof. Schmelcher, what do you consider the core tasks of a graduate school?

One of the main tasks of our graduate school is to provide an excellent educational program to enable the PhD students to perform excellent research in their individual research groups. Apart from the course program with its various modules this is supported also by a strong, meanwhile very well established, guest program and many opportunities for the students to travel to meetings, workshops and conferences. Building up a scientific network is an important step in today's research world for an academic (or non-academic) career. This serves not only the purpose of being updated with the most recent developments and to acquire the most recent technology in your specialized research field, but also to meet the leading experts personally, knowing them and becoming known by them due to one's research expertise. In todays research the number of publications appearing daily is enormous and hard to follow, which is why this ,channel' of dissemination of research results has become increasingly important over the past years. Our graduate days represent an excellent platform in this respect since the courses offer the opportunity to ask individual questions and to personally discuss with the lecturers, who are leading experts in their fields.

What is the difference between the CUI Graduate School and other graduate schools?

From the very beginning it was clear that one of the challenges of CUI and in particular of the CUI graduate school will be to find a common language: CUI covers research wise the full span from physics and chemistry to structural biology and selected medical applications. As such it is truely interdisciplinary and, in view of the specialization in individual research groups, it is by no means easy to find a common platform and ground for discussions and interactions.

What worked out especially well in this context over the past five years?

We have been trying hard to push on this frontier and, this is my impression, we have indeed been successful to some extent. Unexpectedly, but at a second glance very naturally, measures such as the winter school of the early career researchers have been instrumental in putting this forward. The winter school is organized by the PhD students themselves, which means that they can decide what is necessary and adequate to learn and progress along the above lines. They decided to go for a mix of presentations on their own research results combined with young invited speakers that cover specific research lines and indeed bridge between the fields of research of CUI. This way the winter school has emerged as a crucial way of binding together the CUI graduates and learning about each other's expertise.

How could CUI's Graduate School develop in the future?

In the future, in particular to further promote the knowledge of each other's research fields resulting in cross disciplinary projects, one could think of several innovative measures. One of them are the so-called idea factories where young researchers come together e.g. in an intense science hackathon at the interface between rigorous academic research and free interdisciplinary exploration. This could serve the purpose to specifically develop and address questions between the specialized fields and to fully exploit any kind of synergies.

What kind of advice for their future would give the graduates?

My personal advice number one has been always to follow your own interests and to take yourself seriously in what you are indeed interested in. It is only this way that you will develop your full potential and will take the deepest satisfaction from what you are doing and what you will accomplish. Sometimes this goes smoothly, other times it brings you to face with the troubles of life that can become a seed for growth.

Thank you very much for sharing these insights.



Winter school on the Island of Ruegen. The school is organized by the PhD students themselves and gives them a good opportunity to present their projects

Molecule Cluster

Few

BUILDING BRIDGES BETWEEN RESEARCH FIELDS

Workshop by and with young scientists – important feedback on one's own scientific work

n June 2016, CUI's graduate school invited participants to a Young Researchers Workshop for the first time. Following Professor Peter Schmelcher's initiative, the workshop's goal was to establish contacts with other PhDs and postdocs from renowned groups and to provide opportunities to discuss and exchange selected topics from CUI's research area A.

Under the title "From few-to many-body physics in cold atomic quantum matter", the young scientists discussed the behavior of quantum systems at the transition from few to many particles.

"We did not have any experience with this kind of concept and are very happy that the liberally planned discussions were well accepted," says Johannes Schurer, who organized the workshop together with Bernhard Ruff, Simos Mistakidis and Christian Fey. "The students received important feedback on their own scientific work. In the meantime, the Each speaker talked for 40 minutes and afterwards the workshop helped to build bridges between the research fields." presented results were discussed for 20 minutes. On the one

Doing your PhD at CUI: lively exchanges, new projects

As of March 2017, 84 PhD candidates were doing research within the cluster of excellence, among them 22 female scientists. Dr. Sabrina Zinn and Dr. Robin Schubert were among the first to complete their PhD at CUI in the year 2016. We asked the two scientists, who worked for the Max Planck Institute for the Structure and Dynamics of Matter and the Institute for Biochemistry and Molecular Biology at Universität Hamburg, about their experiences.



Sabrina Zinn: At the end of 2012 Melanie Schnell offered me a move to CUI. You would not say no to such a great opportunity! The most valuable experience during my time at CUI was to get in contact with other PhD candidates and research fields and to exchange ideas. In addition, I could participate in a broad travel program and meet with

scientists who are interested in my work in particular. That was really nice. And I really enjoyed participating in the graduate days and the summer and winter schools.



hand, this concept allowed speakers to provide sufficient details from their work, on the other hand, there was enough time for the participants to discuss the topics, so that they could connect the respective working groups and their particular methods.



Robin Schubert: When you graduate at CUI, you do not disappear in your lab for three years. Instead, there is a lively exchange with other research groups. You can discuss your ideas with others and then develop them further. I also enjoyed taking part in the winter schools and in the graduate days. On a couple of occa-

sions, mutual research projects developed from those discussions. Conferences and workshops which were financed by CUI have also stimulated my research.

FOCUSING ON RESEARCHERS **IN NEED**

PETER SCHMELCHER SUPPORTS THE **COMMITTEE ON INTERNATIONAL** FREEDOM OF SCIENTISTS (CIFS)



he freedom of research is not always given as it is in Germany. When scientists are hindered in the pursuit of their scientific interest, this is a case for the Committee on International Freedom of Scientists (CIFS) of the American Physical Society. Professor Peter Schmelcher, Director of the CUI Graduate School, was a member of the globally active committee from January 2014 until December 2016. The committee is responsible for monitoring concerns regarding human rights for scientists throughout the world, especially concerning the freedom of research activity. Key aspects of its mission are the representation of the interests of the person concerned towards authorized institutions and political decision-makers as well as generating highly visible publicity on the cause and the individual situation.

Reliable information

"The cases that the Committee is engaged with can be rather complicated and an important first step is to achieve reliable and complete information," Schmelcher explains. Nine members of the committee meet twice a year in Washington to discuss the cases and to define a strategy. It can be emotionally stressful, admits Schmelcher, and describes the situation of the Iranian physicist Omid Kokabee as a typical case:

Kokabee conducted research at the Institute of Photon Science in Barcelona from 2007 to 2011 and then at the University of Texas at Austin. During a visit to Iran, he refused to work for military research there. He was then prevented from leaving the country and sentenced to ten years in prison by the revolutionary court on charges of "communicating with a hostile government (USA)" and "illegitimate/illegal earnings". A number of institutions started a public campaign to draw attention to the researcher's fate. They wrote petitions and articles were

published in the New York Times. Furthermore, Kokabee was awarded the Andrei-Sakharov-Prize of the American Physical Society. An initiative involving top-level political decision-makers in the USA achieved Kokabee's transfer to a hospital; he was released on parole in 2016 after having served more than five years in prison.

Hard conditions in prison

"Despite very hard conditions in prison, Kokabee refused to give in to the Iranian demands and fought heroically," Schmelcher emphasizes. Schmelcher, who is the leader of the Theory Group of Fundamental Processes in Quantum Physics at the Centre for Optical Quantum Technologies of Universität Hamburg, had thought thoroughly about his engagement. He was pleased when the committee's chairman, who had heard him take a strong stand during a discussion in Harvard, contacted him. "Of course I want to help in difficult situations. The question is, whether you are the right person," Schmelcher says. The members are elected for three years.

For almost 30 years, the CIFS has supported scientists in need. The Committee investigates human rights abuses, gathers information, supports the persons affected, and informs colleagues and the public. "The freedom to research and teach as we know it from Germany is suppressed in other countries," Schmelcher says. The committee is not politically active but stands up for individual cases. "We take the initiative when researchers lose their position or are threatened by imprisonment. Very often the individual situation is an indicator for the general situation in the respective countries," he explains. In some cases the situation can be changed, but this is not predictable. Somebody who is involved in this way has to have a very open motivation. But Schmelcher says: "The persons affected are very thankful." 🗖

SCHOOL LABORATORY OFFERS EDUCATION **PROGRAM FOR FUTURE TEACHERS**

INSPIRING PUPILS AND BOOSTING TEACHERS' SKILLS

dvanced training enables students to dive deeply into experimental work und look into current research. Prof. Erika Garutti from the Institute of Experimental Physics at Universität Hamburg, who coordinates the so called F-Praktikum, and Professor Klaus Sengstock, who is the director of "Light & Schools" initiated a new offer to bring both areas closer together.

The school laboratory, which is financed by CUI, aims to build a bridge between school and research. By offering newly developed and exciting experiments, coordinators Bastian Besner and Dr. Monika Kobylinski hope to spark an interest in physics among young people. Pupils can develop their own app, create Liquid Crystal Displays, work with GPS systems and build their own speakers. The projects are often connected to everyday objects like mobile phones, loud speakers or 3D cinemas, and they usually try to appeal to aesthetic aspects. In their last years at school the boys and girls have the opportunity to learn about lasers and coherent light, they can visit scientific talks and join lab tours. In this way, "Light & Schools" wants to open new doors to the natural sciences.

The F-Praktikum offers a broad range of experiments, which give strong insights into modern experimental physics. "This is perfect for future scientists. Future teachers, however, have told us that it can be a problem for them to enter so deeply into the science," says Dortje Schirok, who was a coordinator at "Light & Schools" until July 2018. Now Bastian Besner and Milan Zvolký have developed a program exclusively tailored to the needs of future teachers. Within the advanced internship at "Light & Schools", students can select an experiment about lasers and coherent light from the program, become acquainted with the theory, develop a didactic concept and then carry out the experiment with a small group of six pupils. Here the motto is learning by teaching, says Garutti.

At the beginning of 2019, "Light & Schools" and the "F-Praktikum" will move even closer together in a new

"Light & Schools"-Team

Prof. Klaus Sengstock is the director of "Light & Schools", the director of the Institute of Laser Physics, and a spokesperson of CUI. He initia-



versität Hamburg where she gained her first teaching experience and completed her PhD in physical chemistry. She

Dr. Monika Ko-

bylinski studied

chemistry at Uni

ted the school lab nine years ago and greatly looks forward to the new building. joined the team in March 2018 and





200 people, among them many pupils and students, joined the ground-breaking ceremony and had a glimpse at the plans of the transparent new building, which was designed by Hammeskrause Architekten

common building. The foundations for the "HAUS DER LEHRE – LIGHT & SCHOOLS" were laid at the beginning of 2018. It is a one-storey, multifunctional and transparent building where pupils and students can profit from each other's knowledge and learning. With 1,070 square meters, the building designed by Hammeskrause Architekten offers space for labs and seminar rooms. Even recreational areas will be equipped with physics experiments. "You can have fun with physics during breaks," Garutti says. "We want to build bridges between schools and the University, between research and teaching," emphasizes Sengstock. The new building will expand Universität Hamburg's presence on Campus Bahrenfeld. The costs of € 3 million will be financed by the University via the higher education pact (Hochschulpakt). This is the first building which the University has realized through its own financial means and using its own building section: UHH Construction Management.



Bastian Besner joined "Light & Schools" as a mas ter's student and started work as a coordinator in 2016 after obtaining his physics degree. His focus is on the new offer for future



teachers, the Codeweek, MINT Pink, and supervises the projects for grades 5-10. the development of new experiments.

THE ACTION PLAN IS BEARING FRUIT

ive years ago, CUI launched an ambitious action plan to make a mark – for men and women. A family-friendly university is everybody's concern, as Prof. Heinrich Graener, Dean of the Faculty of Mathematics, Informatics and Natural Sciences at Universität Hamburg, then stated. The action plan has two principal aims: first, to create better opportunities to balance a scientific career and family life and second, to support female scientists at all levels of a scientific career. "Whether we will achieve our aim of increasing the share of women in natural sciences will only become evident within a few years. A lot will have to change in the heads of decision-makers," Professor Melanie Schnell said, who represented equal opportunities in the CUI board from 2013 until 2017. "But what we can see is that our programs have been established and more and more women scientists are put forward for our awards and fellowships."

The Mildred Dresselhaus Guest Professorship Program

comes with prize money and a teaching and research visit at CUI and is awarded to one senior and one junior extraordinary woman scientist every year."This works in two directions," Marie Lutz, who is the Equal Opportunity Officer at CUI, explains. "The senior scientists bring along their prestige and know-how which we profit from here in Hamburg. The junior scientists then again seem to reap enormous personal benefits and get a real kick for their career."

The organizing team of the "Mildred Dresselhaus Guest Professorship Program" at CUI has even been honored with the Equal Opportunity Prize 2018 of Universität Hamburg in recognition of its particular commitment to empowering (young) female scientists in physics and the positive effects on the whole science community. The prize is worth € 10,000.

The Louise Johnson Fellowship kicks in at an earlier stage in the scientist's the career: it offers a two-year position to a female postdoc. "More and more CUI scientists - men and women – take this chance to reward and encourage a good junior scientist with an attractive position," Lutz explains. Above all, internal as well as external applicants profit from this.

Furthermore, CUI and a number of partners invite women to the twice-yearly Women's Career Day that offers workshops on career-related subjects. An evening program has been added which generally deals with the topic of equal opportunities and also explicitly addresses men. In line with the title "Gender, Neo-Liberalism and Research in a Global Knowledge Society", Prof. Louise Morley, director of the "Centre for Higher Education & Equity Research" (CHEER) at the University of Sussex, outlined the consequences of neo-liberalism at the kick-off event. Lutz: "We want to see our topics in a broader context and therefore need ideas from all kind of directions." The same is true for the annual event called Scientific Career and Parenthood which provides an opportunity for scientists at all career stages to discuss the legal framework and come up with practical strategies to balance their family lives and careers.

The Academic Leadership Program for Women explicitly addresses postdocs and junior professors. This workshop series focusses on the self-perception of one's leadership competence, effective leadership behavior and the preparation for future leadership positions. The program also aims to boost the interdisciplinary networking with scientists from University Medical Center Hamburg-Eppendorf (UKE) and the MIN Faculty of Universität Hamburg.

A mentoring program designed especially for women on Campus Bahrenfeld has also been initiated. dynaMENT Mentoring for Women in Natural Sciences is a joint project of CUI, DESY, the collaborative research centers SFB 676 and 925 as well as the PIER Helmholtz Graduate School. Its target groups are PhD students and postdocs of the participating institutions (see page 21).

Another highlight was the 20th Women in Physics Conference under the patronage of the Federal Minister of Education and Research in November 2016, following an initiative by CUI. Apart from the professional exchanges, the networking of women physicists from all qualification levels - ranging from bachelor students to professors and industry physicists - was an important goal. A panel discussion with Hamburg's Science Senator and Second Mayor, Katharina Fegebank, was chaired by CUI Equal Opportunity Officer Marie Lutz and offered the chance to look beyond the boundaries of each profession. In addition, CUI and DESY jointly prepared a special program for schoolgirls.



The organizing team of the "Mildred Dresselhaus Guest Professorship Program" at CUI has been honored with the Equal Opportunity Prize 2018 of Universität Hamburg. The prize is worth € 10,000 and was presented by Vice President Prof. Jetta Frost (right)



The kick-off event was also a thank you to the mentors and celebration of the mentees of the 2017/2018 round, who are holding their certificates

dynaMENT Mentoring Program for Women in Natural Sciences

n PhD research, one is going where there is no trail, exploring new territory," Professor Dwayne Miller, director at the Max Planck Institute for the Structure and Dynamics of Matter and spokesperson of CUI, said at a kick-off event of the mentoring program. "One needs a good guide to get you through," he added. "dynaMENT - Mentoring for Women in Natural Sciences" wants to provide precisely this career compass to female PhDs and postdocs who are planning to

work in academia.

The program started in 2015 as the first campus-wide The mentors are excellent researchers at advanced career mentoring program for women in the natural sciences in levels: professors, group leaders, senior scientists, scientific Hamburg-Bahrenfeld. In 2017 it received its name, "dynaMENT coordinators. In parallel to the program for the mentees, Mentoring for Women in Natural Sciences". Most of the parthey are trained by an external coach as well. "We hope that ticipants highly appreciate the consultations with their menmentors and mentees meet up as much as is possible and tors. "It is a great opportunity to be a mentee, because I can necessary in addition to the events," Ostermaier-Grabow says. Mentor and CUI Professor Arwen Pearson (Universität profit from the experiences a successful female scientist has made. Thanks to my mentor's support I get deep insights into Hamburg) builds upon her own experiences: "I was lucky the scientific landscape. It is of high value for me to discuss enough to have, and still have, great mentoring. So this is the feasibility of my career goals and my scientific plans with my way to pay things forward - and it is very rewarding to my mentor," says Dr. Antonia Karamatskou, a CUI fellow and see someone grow." mentee of the first round in 2015/2016, who was coached by Mildred Dresselhaus Guest Awardee Professor Anouk Rijs. "Seeking advice is a sign of strength," emphasizes Professor dynaMENT in short Daniela Pfannkuche, executive director of the Institute of Theoretical Physics at Universität Hamburg,

The candidates have to participate in a comprehensive application process to be accepted in the program. But, as Miller says: "When you leave this program, you can do it - no matter what comes." dynaMENT offers confidential one-toone sessions with experienced female mentors from various scientific fields, networking events and workshops in English. Shortly after the kick-off, the first workshop for mentees is usually moderated by Anika Ostermaier-Grabow. "It is mostly a very lively afternoon. They are all there and very curious



"IT IS VERY REWARDING TO SEE SOMEONE GROW"

about the stories the others have to tell and eager to exchange ideas," the project manager and program organizer says. This session is followed by several further workshops with external trainers which are then supplemented by networking events on topics that are tailored to the workshops. These include strategic networking, conflict management, diversity & intercultural challenges, job Interview /self-presentation, self-marketing & search committees and leadership skills. The series ends with a reflection process.

dynaMENT is organized jointly by CUI, DESY, the Max Planck Institute for the Structure and Dynamics of Matter, the MIN Faculty at Universität Hamburg, the PIER Helmholtz Graduate School, and the Collaborative Research Centers SFB 676 and 925. The program is designed for a period of 12 months and held in English. At the end, the participants receive a certificate for their participation which also lists all the events they attended.

EVENTS





Above: You can hear and see it from far away: In the sound sculpture "Unit Cell" sound waves hit the balls

Left: Fascination for physics: Prof. Gunter Huber (Institute of Laser Physics) tirelessly explained the laser exhibits

THE SOUND OF CRYSTALLOGRAPHY

EXPERIENCE SCIENCE WITH ALL YOUR SENSES

s it possible to hear crystallography? The members of the arts group "The Superposition collective", Lawrence Molloy and Dominic Hopkinson, gave it a try, together with scientists Professor Ben Whitaker and Dr. Mike Nix of Leeds University. The result is a sound installation that appeals to all our senses. For the Night of Knowledge 2015, CUI and the Center for Free-Electron Laser Science arranged for the exhibit called Unit Cell to be reconstructed and put in front of the CFEL building as an eye catcher.

"One hundred years ago the physicists William Lawrence Bragg and William Henry Bragg first worked out how to investigate the structure of crystals with X-rays," Professor Arwen Pearson of Universität Hamburg explains. She brought the exhibit to Hamburg to show it during the Night of Knowledge. Inspired by the more than 100-year-old scientific work, the X-rays were substituted by sound waves; 125 balls arranged in a threedimensional lattice symbolize the crystal. As soon as the sound waves hit the balls, a sound field arises that fills the room around the sculpture - sometimes it is loud, at others quiet. It makes the research field of crystallography sensually perceptible.

The Unit Cell is an example of the engagement and creativity that scientists possess in trying to make their research accessible to everyone. The great interest of visitors reinforces their efforts: more than 18,000 people used the Night of Knowledge and DESY's open day to get further insights into the many research facilities on the Campus Bahrenfeld. The Unit Cell is now a permanent exhibit in the atrium of the CFEL building. ■

FRESH KNOWLEDGE FROM THE TAP

"Can nanoparticles cure?" That was the question Professor Horst Weller (Universität Hamburg) asked the audience in a bar in Hamburg's Sternschanze district. "What do we need them for and will they maybe help to defeat diseases?" With that, he sparked off a lively discussion, just like Professor Franz X. Kärtner. The fourth edition of "Wissen vom Fass" (Science on tap) again gave the public fresh insights into science and the lives of scientists.

This year's talks ranged from STEM, the humanities and social sciences through to legal sciences. Forty-five scientists spared no effort to explain their highly complex research - sometimes in small groups with six people, sometimes with 100 guests, sometimes as an exquisite discussion round, in other cases as a scientific happening.



"How do you shrink an accelerator?" Prof. Franz X. Kärtner (Universität Hamburg, DESY, MIT) asked his audience

"Wissen vom Fass" is jointly organized by DESY, CUI, the collaborative research center Particles, Strings and the Early Universe (SFB 676), the Department of Physics at Universität Hamburg, and PIER, the strategic partnership between DESY and Universität Hamburg.

THE BEAUTY OF SCIENCE

GREAT SUCCESS FOR "ARTS & SCIENCE" IN HAMBURG'S CITY HALL



veryday life as a researcher is characterized by pionee- ring spirit and scientific focus. "Only rarely does one change one's point of view. If you do, there is an incredible diversity," Prof. Peter Schmelcher (Universität Hamburg) said opening the exhibition "Arts & Science" first shown in the summer of 2017 in the foyer of Hamburg's City Hall.

The exhibition originated in a contest among memstressed: "It is good that you show that a discipline like phybers of CUI. What makes it so special is that it is not the sics, which appears quite sober at first glance, can look as it scientific impact that counts, but - instead - the aesthetics. does." He was curious to hear about the impact for artists. This approach was quite right for the two-week exhibition: thousands of people visited City Hall, surveyed the vibrant "Art can make science understandable, while at the same pictures, let themselves be attracted by the colors and - by time science enables art to work," Prof. Julia Lohmann, who reading the accompanying texts and looking at the lab was involved in selecting the pictures for the exhibition, photos - gained new insights into basic research in the explained. Her professional focus is on connecting science natural sciences. Due to the great resonance the pictures and artistic creativity. The fruitful collaboration was a great were even shown a second time in City Hall. success for CUI.

Pas de Deux: On the interplay between art and natural science

Even though the methods of examination and the language differ, art and natural science cannot be separated from each other. On the contrary: as if in a dance they develop a relationship and influence each other.

The progress in the natural sciences, especially in physics and chemistry, is driven by the quest for knowledge and understanding as well as the search for the fundamental principles which are responsible for nature's complexity.

In addition to the scientific quest for insights, the natural sciences offer an impressive beauty which shows up in many visualizations and offers a fascinating aesthetic view of science.

Arts and science may offer two different paths towards the understanding of our world, but they do have an

Science expands our senses, it lets us see microscopic worlds and solar systems, understand historical events and recognize parts of the future. It forms our understanding of ourselves and the world which surrounds us. It influences our actions, our dreams and our striving – and therefore our art and design.



"Thank you very much for the great research results, thank you very much for the public event," Dr. Rolf Greve, Director-General at the Hamburg Ministry of Science, Research and Equalities, said at the opening. "We should try to do more in this direction, because we need such events to show the public how beautiful science can be."

Prof. Dr. Dieter Lenzen, President of Universität Hamburg,

influence on each other. The overlap is the astonishment, the desire to understand things and learn new ones, sparked by something beautiful, special or unknown. The astonishment leads us to ask further questions and explore more deeply. Visualizations fill abstract physical principles with life and make the research accessible to a wide audience.

By Prof. Peter Schmelcher and Prof. Julie Lohmann for the exhibition poster "Arts & Science"



Prizes and awards IV.



Dr. Denise Erb (former CUI) has been awarded a Prize by the Association of the Friends and Sponsors

of DESY for her outstanding PhD thesis (2015).



Prof. Gabriel Bester (UHH) has been honored by the High Performance Computing Center Stutt-

gart (HLRS) with the traditional Golden Spike Award 2015.

Hamburg Prize for Theoretical Physics 2013-2017

From 2013 - 2017 CUI and the Joachim Herz Stiftung have jointly awarded the "Hamburg Prize for Theoretical Physics" to five outstanding physicists. The prestigious prize worth € 40,000 honored outstanding contributions of a highly accomplished international researcher in the field of Photon Science, especially Quantum Optics, Laser Physics, Ultrafast Physics, and X-ray Physics:

2017 - Prof. Dr. Andrew Millis, Columbia University, Simons Foundation, New York, USA

2016 - Prof. Dr. Mikhail Katsnelson, Radboud-University, Nijmegen, Netherlands

2015 - Prof. Dr. Ignacio Cirac, Max Planck Institute of Quantum Optics, Garching, Germany

2014 - Prof. Dr. Antoine Georges, Collège de France, École Polytechnique, Paris, France, and University of Geneva, Switzerland

2013 - Prof. Dr. Chris H. Greene, Purdue University, West Lafayette, USA

DOI:10.1016/j.chembiol.2016.06.008

burg.de/en/events/arts-and-science/

European XFEL

From 2018 on the prize will be awarded by CUI and the Joachim Herz Stiftung together with the Wolfgang Pauli Centre (WPC) of Universität Hamburg and DESY as a new partner. It involves now all areas of theoretical physics and is endowed with a prize money of € 100,000.

> A team of scientists led by Prof. Henning Tidow (Universität Hamburg) determined the structure

of a thiamine transport protein - an important

milestone in membrane transport research and

The photo shows a sample right before it is locked

into a scanning tunneling microscope operated by

the group of Professor Sebastian Loth (MPSD, Uni-

versität Stuttgart) at the Center for Free-Electron

Laser Science. The scanning tunneling microscope

for drug discovery in the long run as vitamin

transporters are responsible for the uptake of essential nutrients

in bacteria. The team made use of lipidic-cubic phase X-ray

crystallography complemented by coarse-grained molecular

mine the illustrated structure of YkoE with bound thiamine.

images materials with extreme magnification and resolves

individual atoms on the material's surface. Unlike conventional

mechanically and generates the image step by step. The photo

was taken for the Arts & Science exhibition. www.cui.uni-ham-

light microscopes, an atomically sharp needle probes the surface

dynamics simulations and fluorescence spectroscopy to deter-

OUR COVER



The illustration shows the setup for a quantum simulator to image the electronic structure of molecules. Scientists from the group of Professor Klaus Sengstock (Universität Hamburg) simulated a benzene molecule, in which a laser field

(bottom) takes the role of the atomic nuclei. This laser field results from overlaying a strong laser beam (red) with an optical lattice. Ultra-cold atoms mimic the electrons in a molecule and allow to imaging an artificial molecular orbital – which makes the distribution of electrons visible (center). *DOI: 10.1103/PhysRe*vX.5.031016



Superfluidity is an amazing dynamic phenomenon of the quantum world: an object which is dragged through a normal fluid experiences friction. However, when it is dragged through a Bose-Einstein condensate there is no friction.

The groups of Professor Ludwig Mathey and Professor Henning Moritz (both Universität Hamburg) together with Professor Jean Dalibard (Collège de France, ENS Paris) analyze the superfluidity of ultracold quantum gases. The illustration shows a laser beam (green spot) which is dragged through a quantum gas (colored pixels). DOI: 10.1103/PhysRevA.95.043631

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