

NEWSLETTER FEMAHRNBELT DAYS 2014



FEHMARNBELT DAYS:

THE MAKING OF A VIBRANT REGION

The Fehmarnbelt Days offer an exciting opportunity to get involved in the up and coming region Fehmarnbelt, encompassing parts of Denmark, Southern Sweden and Northern Germany. This year's event follows up on the 2012 edition, where more than 600 people came together to join in on discussions and workshops offered by the various stakeholders.

The Fehmarnbelt Days provide a platform for anyone interested in the potential of this vast growing region. The list of participants ranges from representatives of science, research and education to politics and tourism. This is a great chance to network and make connections across borders and businesses. It is expected that some discussions led by high level panellists, such as the discussion on innovation in sciences and regional development co-organised by the Roentgen-Angstrom-Cluster, will contribute to achieving concrete ideas as to what a scientific cooperation could look like and why it might add to the region's competitiveness.

Geographically, the region will grow closer through improved transportation and infrastructure over time. It is expected that the opening of the Fehmarnbelt crossing, planned for 2021, will have a major impact on the region at large and the nine million people living in its closer proximity.

The Fehmarnbelt Days are one step ahead of the logistics: the organisers aim to build on existing networks and crossbroder activity and initiate new ideas, so that the region will soon become a prime example for a vibrant, international community that takes advantages of its location and is driven by a variety of actors from different backgrounds working together to move forward.

ABOUT US

FACTS ABOUT THE RÖNTGEN-ÅNGSTRÖM-CLUSTER

The Röntgen-Ångström-Cluster is a collaboration between Germany and Sweden on utilizing synchrotron and neutron radiation in the fields of materials research and structural biology.

Following the decision of various European partners to build the European Spallation Source (ESS) in Lund (Sweden), representatives of the German and Swedish governments signed a Memorandum of Understanding detailing their commitment to future collaborative projects. Both countries made clear they want to work together very closely on utilizing synchrotron and neutron radiation in the fields of materials research and structural biology. The collaboration was given the name Röntgen-Ångström-Cluster.

The Röntgen-Ångström-Cluster includes several research centres: the research centre DESY in Hamburg with PETRA III and FLASH, the Helmholtz-Zentrum Berlin for Materials and Energy (HZB) with BESSY II and BER II, and Helmholtz-Zentrum Geesthacht (HZG). These institutes, together with the synchrotron radiation source MAX IV, currently under construction in Lund, offer researchers of the region outstanding research possibilities in the field of materials science and structural biology. With the X-ray laser European XFEL, currently under construction in Hamburg and with DESY's strong participation in the planned European Spallation Neutron Source in Lund, the range of facilities will be extended to include world-leading photon and neutron sources.

The Editors

EXCLUSIVE INTERVIEW

SIn a first ever interview together, Helmut Dosch, Chairman of the DESY Board of Directors, and Ulf Karlsson, Professor at the KTH Royal Institute of Technology, talk about the purpose and aims of the German-Swedish collaboration.

RÖNTGEN-ÅNGSTRÖM-CLUSTER: INTERNATIONAL POWERHOUSE AND A MODEL FOR EUROPE



What is the purpose of the Röntgen-Ångström-Cluster?

Helmut Dosch: In view of the excellent research infrastructure such as the brilliant X-ray sources and the neutron sources that are put in place in Hamburg and in Lund, it became evident that both countries, Germany and Sweden, have to work much closer together. After there has been prominent focus on the infrastructures in the past, the Röntgen-Ångström-Cluster allows us now to better emphasize research. By joining forces we will make the best scientific use out of these outstanding facilities.

Ulf Karlsson: I personally have come to Hamburg since 1980 to pursue research. There has been a long tradition by Swedish scientists to use DESY's research facilities. Now we want to broaden and deepen this collaboration in a structured way by working together very closely on utilizing synchrotron radiation and neutron sources in the fields of materials research and structural biology – fields where our research facilities offer excellent research opportunities.

Would you say the Röntgen-Ångström-Cluster stands out from other collaborations?

Ulf Karlsson: It was a rather unusual decision for Sweden to collaborate with one specific country only and one has to give credit to the Swedish government to establish this novel collaboration structure. The Röntgen-Ångström-Cluster is indeed very unique and we have already received many applications and project proposals from German-Swedish research teams. **Helmut Dosch**: The Röntgen-Ångström-Cluster is a whole new strategic cooperation. It demonstrates that something has changed on the governmental level. It shows that ministers understand that any future development requires the promotion of science and research at the core level and strategic cooperation with partner countries on a bilateral or multilateral level.

What are you hoping to achieve?

H. Dosch: We would like to become an international powerhouse and create a European Centre of excellence in Northern Europe. Eventually this German-Swedish collaboration of joint funding and joint programming could be a role model for other research-intensive regions in Europe.

U. Karlsson: In fact, we are also open to international partners. We have had talks with several other countries and the Röntgen-Angström-Cluster can be a model for the Baltic Science Link. Other countries can join as long as they participate in co-funding the research programmes. Science does not know any national borders.

(photo: Helmut Dosch (I.) and Ulf Karlsson, © K. Strobel)

Starting with this edition, we aim to introduce some of the projects supported by the Röntgen-Ångström-Cluster in each newsletter to come. If you are working on a project and would like to share your progress, please contact us at editor@rontgen-angstrom.eu.

DIMETAL-CARBOXYLATE CATALYSIS IN ENZYMES AND BIOMIMETIC MATERIALS STUDIED BY NOVEL X-RAY CRYSTALLOGRAPHY AND SPECTROSCOPY TECHNIQUES



Project Partners: PD Dr. Michael Haumann (Coordinator), Freie Universität Berlin; Prof. Volker Schünemann, Technische Universität Kaiserslautern; Prof. Martin Högbom, Stockholm University; Dr. Sascha Ott, Uppsala University

Proteins containing transition metal cofactors are of outstanding biological relevance. Their biological reactions are of prime

interest also for technical applications in renewable energy, chemical industry, and medicine. A cofactor containing two metal ions coordinated by carboxylate groups in a highly conserved amino acid fold (dimetal-carboxylate cofactor, DMC) defines a large and diverse superfamily of proteins. DMC enzymes perform some of the chemically most demanding reactions in nature, for example the selective oxidation of methane to methanol, listed among the top-ten challenges for catalysis. Prominent members of the group are ribonucleotide reductases involved in DNA synthesis and monooxygenases with widespread substrate specificity. Mimicking the green chemistry of these systems is an outstanding goal for bioinorganic and organometallic chemists. Our understanding of the molecular, electronic, and vibrational properties of DMCs at present is insufficient to explain their various functionalities.

The archetypical DMC consists of two iron atoms (FeFe), but very recently, enzymes have been discovered, which instead bind MnFe or even MnMn cofactors. Their primary function is similar, namely activation of O2 at the entry point of electron transfer, radical formation, and substrate oxidation reactions, involving crucial reaction intermediates with high-valent metal ions. The reasons for the different metallations of the binding sites, as well as the structural and electronic differences

COFACTOR

A cofactor is a non-protein chemical compound which is required for the biological activity of a protein. These proteins are commonly enzymes, and a cofactor can be considered as helper molecules that assists in biochemical transformations.

REDOX

"Redox" comes from REDuction and OXidation and refers to atoms' change of oxidation state in chemical reactions. In electron transfer, a reduction is a decrease in oxidation state by a molecule, ion, or atom which causes a gain of electrons, whereas oxidation means the increase in oxidation state which makes a loss of electrons. between them are widely unclear. In the trans-disciplinary project, we aim at gaining deeper insight in the reaction mechanisms of the biological systems that potentially will lead to new biomimetic catalysts by linking structural biology and functional organometallic materials with development and application of novel synchrotron-based X-ray crystallography and spectroscopy techniques.

Experiments at the new facilities PETRA III (DESY, Hamburg) and MAX IV (Lund, Sweden), as well as at free electron laser sources are combined to obtain complementary information on reaction intermediates. X-ray absorption and emission spectroscopy (XAE) provides electronic configurations and fine structures. Nuclear resonance scattering (NRS) on isotopically labeled systems discloses vibrational dynamics and protonation events at the cofactors. Free electron laser femtosecond protein crystallography (FFC) will be employed to obtain molecular structures of high-valent states of wildtype and mutated proteins. Synthetic chemistry is used to implement the crucial features of the biological systems into tailored molecules. We will improve the instrumentation at two beamlines (P01 and P64) of PETRA III for a broader user community and gain experience on the application of free electron laser experiments to high-valent metal centers in proteins to be used at the upcoming sources (European XFEL, MAX IV). Integration of the spectroscopic and structural data with guantum chemical calculations will yield atomic-level models and reaction mechanisms for the DMC systems. This unprecedented information will significantly improve our fundamental understanding of the metal specificity, redox tuning, and functional diversity of this class of transition metal catalysts.

NEWS

A Swedish-German research team has successfully tested a new method for the production of ultra-strong cellulose fibres at DESY's research light source PETRA III. The novel procedure spins extremely tough filaments from tiny cellulose fibrils by aligning them all in parallel during the production process. The new method is reported in the scientific journal Nature Communications and you can read more about it at http://www.rontgen-angstrom.eu/go/cellulose

PROJECTS

CONTROLLING SAMPLE INTEGRITY IN FEL EXPERIMENTS: Exposure, heating, and plasma dynamics in the time domain Project Coordinator: Prof. Maria Krikunova, Institut für Optik und Atomare Physik, Technische Universität Berlin, Germany; Dr. Jakob Andreasson, Department of Cell and Molecular Biology, Uppsala Universitet, Sweden







ty to arrange sample particles in large high-quality crystals. Instead, scientists will be able to study structure and dynamics in complex biomolecules directly.

Due to the high power density of the FEL radiation needed for high resolution Coherent Diffractive Imaging (CDI), the sample will be turned into a highly excited plasma after exposure. Thus, the electron dynamics eventually followed by the ion displacement in the sample during the pulse directly affect the formation of the diffraction pattern and put an ultimate limit to the obtainable resolution. Furthermore, the sensitivity of structure and function of biological samples to changes in their environment requires new concepts for sample delivery and precise control under high vacuum conditions.

The four-year research program within the Röntgen-Ångström-Cluster will refine the sample-delivery techniques that allow for handling of inorganic, organic and biological nanostructures. It will also develop the time-resolved methods to track the dynamics of nanometer- to micrometer-sized plasmas on ultra-short time scales.

Within the collaboration we will focus on the development of: (i) a cluster source for production of water nano-particles which could be doped with a variety of substances, including proteins and other macromolecules;

(ii) a sample delivery system capable of trapping and manipulating individual droplets in an interaction region where they can be held captive during the exposure;

(iii) key experimental and theoretical components for the study of the dynamics of nano-plasma formation using terahertz or near-infrared radiation combined with X-ray FEL pulses with high temporal and spatial resolution;

(iv) computer modeling for studies of matter in extreme conditions and methods for handling the vast quantities of data generated by e.g. the European XFEL.

The research project brings together the complementary experimental and theoretical expertise of the research groups from Uppsala and Berlin in the fields of CDI, handling of biological samples and computer simulations to address the development of new time-resolved techniques for studies of ionization dynamics of small quantum systems. The results from this collaboration will contribute to the understanding of the physical processes that govern the response of matter under extreme irradiation conditions. Furthermore, it will enhance the exploration of the full potential of Swedish-German research infrastructures: MAX IV, FLASH as well as the European XFEL.

ANNOUNCEMENTS

SECOND RACIRI SUMMER SCHOOL

The RACIRI summer school is a joint German-Swedish-Russian initiative to promote the next generation of scientists with a strong connection to the large-scale research infrastructures (synchrotrons, lasers, neutrons) in the Baltic area. The first RA-CIRI Summer School on advanced materials design was successfully held in Peterhof, Russia, in 2013. This year's RACIRI Summer School was organized in August on "Imaging with X-rays and Neutrons in Life and Materials Sciences" in the greater Stockholm area, Sweden. To read a summary, please visit our website us on www.rontgen-angstrom.eu.

FIRST NORDIC X-RAY SCIENCE DAYS Opportunity to get together with the large user community

MAX IV Laboratory announces the first Nordic X-Ray Science Days to take place from 27th of September until the 1st of October this year (2014). Traditionally, MAX LAB IV used to organize the Annual MAX IV Laboratory User Meeting (UM14) in cooperation with The Association for Synchrotron Radiation Users at MAX-lab (FASM). This year, the event has been extended to include a much larger user community. The aim of the Nordic X-Ray Science Days is to engage all Nordic X-ray users and to build more bridges between the various institutions committed to X-Ray sciences. The event takes place in Lund, Sweden, Downtown University Campus.

Please visit www.rontgen-angstrom.eu to get more information.

WE ARE THE COOLEST SHOW IN TOWN Christoph Quitmann about the MAX IV facility in Lund



MAX IV has just started to commission the linac. Are you pleased with your team's work?

Yes, very pleased. The team did a fantastic job. This is the first real step from design to realization. There were more than ten thousand technical issues to be solved, and the team solved them. I'm proud of it.

You arrived in Lund about two years ago from Switzerland. Can you recall your first impressions of your new work place? Yes, I have always found this to be a cool project. Seeing the reality and the people around it was a real revelation. This is the coolest show in town, a landmark. My first impression was real excitement.

How does Sweden compare to Switzerland in terms of work, concerning your particular field?

It's the same, but different. Many things are similar. The technical challenges for example are the same. But the resources in Lund are much more limited. We operate in a different mode. We have a team of 160 people – that is a very small number. Having said that, I'm impressed with the spirit of the people to pull off such a project with limited resources. Another difference is that the facility in Switzerland was located in the woods. In Lund, we're very close to the University. This has an impact on the atmosphere, it's more vibrant.

Tell us about your achievements in Lund so far.

The Linac is operational. The outside of the building is completed. We're working on installing the magnet rings. Most importantly: we managed to build trust and confidence in the Swedish and the international science community. We're no longer a project on paper. People take us seriously. Brasil and Japan, for example, watch us closely and copy some of our methods. We're proud of that but the attention also builds up the pressure.

What are your next challenges?

They are clear. We need to complete the installation and the building. We also have a facility which is currently operating and handling about 1000 users per year until the end of 2015. None of us gets bored.

The new facility is scheduled to open in June 2016. Will it open on time?

Yes, it will. There is no indication of a delay. We are confident to open on Midsummer's Day 2016, Tuesday, 21st of June at 1 o'clock. This is an important time for Sweden. And we realized it was important to have a target date in mind. So we decided to use the brightest moment in the year to open the brightest X-ray source in the world.

How will MAX IV change the scientific landscape?

Already now, MAX IV has had an impact. We're making possible what previously wasn't. We will provide more information with less radiation damage. But it can't be done by us alone. We need the best users from around the world to bring their best projects to Lund.

A personal question: What do you value most about life in Sweden? Is there anything you can't adjust to? Do you find the time to learn Swedish?

I like the people. They are very friendly. I love the Swedish light in the summer. But as a keen mountain biker and climber I miss the mountains. I try to learn Swedish but the Swedish make it very hard for me. Everybody speaks perfect English, so there's little driving force. However, I have recently discovered Astrid Lindgren movies I used to watch as a child in Swedish with English subtitles. That might help me learn.

FIRST ELECTRON PULSES IN MAX IV

WORK ON THE NEW FACILITY WELL ON SCHEDULE

The Max IV facility in Lund, Sweden, has produced its first electron pulses in May this year. "It was great to see that everything worked as it should", said Sara Thorin, project manager for the linear accelerator. Thorin and her team, consisting of numerous scientists and engineers, concluded this part of their mission well on schedule after devoting the past six months to it. The next challenge will be to tune all magnets, radio frequency components, diagnostic and other systems so that electron pulses can be shaped and transported as needed when sent onwards to produce light. Eventually, the electrons will be sent into the storage rings or the short pulse facility.

The large storage ring is expected to be installed in July 2015 and the small storage ring in January 2016. Commissioning of the entire facility is scheduled to commence in the second half of 2015 and the inauguration of MAX IV will take place on June 21st in 2016.



First electrons running at MAX IV: The linear accelerator group has turned up the temperature of the cathode producing electrons in the gun. Everything worked just as it should, and out came the ten longed-for electron pulses per second. Photo: MAX IV

PEOPLE

Rolf Greve: Building bridges across academic disciplines

Mats Johnsson: Promoting International Research Infrastructures



Promoting research in the city of Hamburg and beyond is Rolf Greve's mission. He works for Hamburgs Ministry of Science and Research and has been a member of the Röntgen-Ångström-Cluster Steering Committee since it first started. To him, the Röntgen-Ångström-Cluster represents a continuation and expansion of the scientific cooperation of the Northern federal states that has been evolving over some

time. The states of Hamburg, Schleswig-Holstein, Lower Saxony, Berlin, Mecklenburg-Vorpommern and North Rhine-Westphalia have joined forces in the interest of science and research. Rolf Greve sees it as one of his main responsibilities as a member of the Röntgen- Ångström-Cluster Steering Committee to represent the interests of these states.

Greve stresses that it is not enough, "to exchange views pro forma". "Money needs to be invested" to support the communication between scientists in very practical ways by means of conferences, workshops and other information campaigns. "The scientists within individual disciplines talk to each other regularly. The challenge is to increase the flow of communication between researchers of different disciplines. The added value is achieved by building bridges across various disciplines - for example from physics to chemistry to biology to medicine." This, says Greve, combined with the most up to date facilities at the large research institutes in the Northern region would guarantuee success in research, such as the development of medical remedies.

According to Greve, the wide range of opportunities offered in the context of the Röntgen-Ångström-Cluster across national borders should be made more transparent. Not only largescale equipment but the planned European Spallation Source (ESS) in Lund as well point to numerous possibilities for the scientists in the field of neutron research. New paths will be opened up and establish the north as "one of the leading sustainable innovation regions of Europe", predicts Greve.

MORE NEWS ONLINE

Please check our website regularly. In due course, we will introduce the remaining six German projects approved for funding in the context of the Röntgen-Ångström-Cluster. www.rontgen-angstrom.eu



As a member of the Röntgen-Ångström-Cluster Steering Committee, Mats Johnsson represents the views and interests of the Swedish government. He is senior advisor at the Swedish Ministry of Education and Research responsible for research policies for natural sciences and engineering and for policy and planning. A large part of his work over the past years has been to realize the government's plans to join and initiate

major research in-frastructures.

"The Swedish government has several large infrastructures in the pipeline", explains Mats Johnsson. Two of these, the European Spallation Source (ESS) and the Max IV-synchrotron are to be built in Lund. ESS is a European project. Max IV is a national facility open for scientists from all countries budgeted to about 200 million Euro. Another facility, the SciLifeLab in Stockholm and Uppsala is a facility for large scale gene and protein analyses built as a national facility but naturally open for scientists from other countries. SciLifeLab was formed in 2009 and is now in the upscale phase to full size with a yearly budget of about 100 million Euro.

"The Röntgen-Ångström-Cluster and the collaboration around ESS have opened up the possibilities for closer collaboration with Germany and the facilities that are under construction there", says Johnsson. The Swedish government contributes to the planned extensions to Petra III in form of a dedicated beamline and research groups working in Hamburg together with German research groups. "The hope of the Swedish government is to have closer ties between the German large-scale facilities in Hamburg and in Berlin and the facilities in Lund (ESS and MaxLab) and in Stockholm (SciLifeLab)" says Johnsson concluding that "the Baltic Sea area is with these research centres a world class region in science".

PEOPLE

Interview with Prof. Dr. Wolfgang Kaysser, Scientific Director of Helmholtz-Zentrum Geesthacht



Why is the Helmholtz-Zentrum Geesthacht involved with the Röntgen-Ångström-Cluster?

The HZG is located in Northern Germany and maintains good links with the Swedish scientific world as a matter of tradition. As one of the most important partners in the BMBF-supported ESS Design-Update project the HZG provides essential information in the fields of instrumentation

methods, detector development and sample environment in order to prepare the construction of the ESS in Lund, Sweden. Additionally, the HZG runs the German Engineering Materials Science Center with several beamlines at PETRA III at DESY. For that reason, the HZG offers one of the most significant access points for materials research on large-scale facilities in Northern Germany and is thus a natural partner within the Röntgen-Ångström-Cluster framework.

Where would you place the importance of an international exchange between scientists nowadays and in the future?

Science has always crossed borders and competition takes place at an international level. In this context, the HZG sees itself as part of the world-wide sciences and nurtures an intensive dialogue and cooperation with organisations and individuals on all continents. The Röntgen-Ångström-Cluster ties in perfectly with these objectives because it facilitates collaborations with competent Swedish partners.

What are the opportunities that the Helmholtz-Zentrum Geesthacht provides for scientists?

Within the realm of the Röntgen-Ångström-Cluster the HZG enables scientists to access the materials-scientific beamlines at PETRA III at DESY referred to earlier.

The idea of the HZG is to establish longterm cooperations with external groups on top of the ordinary access via proposals. The objective here is to realize specific complex in-situ sample environments for joint research projects.

The Röntgen-Ångström-Cluster takes up this idea in an ideal way and supports suitable projects with Swedish partners.

Does the Helmholtz-Zentrum Geesthacht run events supporting the objectives of the Röntgen-Ångström-Cluster?

Since 2005, the HZG has been organising an autumn school dealing with materials research and neutron and synchrotron radiation every two years. This school will next take place in October 2013 as one of two R-Å-C-schools and intends to provide Swedish students with in-depth insight into these fields of research. (Photo: Helmholtz-Zentrum Geesthacht)

To find out more about the Autumn School in October 2013, visit www.rontgen-angstrom.eu (section announcements).

Ulrich Lienert: New manager of Swedish Beamline at DESY



Ulrich Lienert's new job as a manager of the Swedish High-Energy Materials Science Beamline at DESY represents a homecoming. The 47-year-old, who took up his position in January 2012, returned to his native Germany after 11 years in the USA and ten years in France. DESY and PE-TRA III, however, are new ground for the physicist.

"This new challenge very much appealed to me. Sweden has a strong materials science community and will have a world class medium-energy synchrotron facility with MAX IV. The Swedish Beamline at the DESY Petra III facility will add world-class high-energy diffraction capability", says Lienert, who gave up his post as Staff Physicist at the Advanced Photon Source at the Argonne National Laboratory in Illinois, USA, to come back to Germany.

Lienert's previous experience seems perfectly tailored to his new job. His first contact with high-energy synchrotron radiation was in the early 1990s, when he researched his PhD thesis at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France, during the construction phase of the highenergy beamline.

He later completed a postdoctoral assignment at the ESRF optics beamline and became interested in high-energy micro-focusing. He became involved in the single grain characterization of polycrystalline materials by means of focused high-energy X-rays and was responsible in this role for the implementation of a first dedicated instrument at the ESRF ID-11 materials science beamline. At the Advanced Photon Source in the USA, Lienert's role was to build up a single grain diffraction programme. This now has an independent user group and, as the scientist explains, "is breaking new ground by involving the strong US modeling community."

In his new job he is aiming at just that: establishing a strong and efficient user group so that the Swedish Beamline at DESY can reach its full potential. "My next step", explains Ulrich Lienert, "will be to visit user groups that have been identified at various universities in Sweden and to find out how the beamline should be tailored to best serve their common interests." He is more than happy to be contacted by potential users: ulrich.lienert@desy.de.



PANEL DISCUSSION DURING THE FEHMARNBELT DAYS 2014

SCIENTIFIC COOPERATION AROUND LARGE-SCALE RESEARCH INFRASTRUCTURES AND THEIR REGIONAL DEVELOPMENT The discussion will be held on 30 September from 16:00 to 17:00 in Copenhagen

During the Fehmarnbelt Days 2014 the Deutsches Elektronen-Synchrotron DESY, KTH Royal Institute of Technology and other members of the Science Link Network, in cooperation with the Röntgen-Ångström Cluster, will hold a panel discussion. The theme will be "Scientific cooperation around large-scale research infrastructures and their regional development". Panellists in the discussion include Pia Kinhult (Governor of Skåne Region, Malmö), Dr. Dorothee Stapelfeldt (Second Mayoress of the Free and Hanseatic City of Hamburg and Senator for Science and Research), Professor Helmut Dosch (Chairman

of the DESY Board of Directors, Hamburg) and Professor Ulf Karlsson (KTH Royal Institute of Technology, Stockholm). We would like to invite you to a lively exchange between scientists, entrepreneurs, politicians and citizens in the Fehmarnbelt region and the whole Baltic Sea area. The three dayevent takes place from the 30 September to 2 October 2014 in Copenhagen at the Tivoli Congress Centre. Key issues are infrastructure, tourism, businesses, labour market, transport and logistics as well as education and research

IMPRINT

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