

NEWSLETTER 11 | APRIL 2015



## NEWS

## GERMAN AND SWEDISH RÅC CALLS OPEN FOR APPLICATIONS

The Federal Ministry of Education and Research (BMBF) and the Swedish Research Council (Vetenskapsrådet) have recently published new calls for research to be undertaken in the context of the Röntgen-Ångström-Cluster. Funding is available for projects involving German and Swedish partners in the fields of structural biology and materials science using neutrons and synchrotron radiation. The deadline for applications is the 29th of May in Germany and the third of June in Sweden. Check out the details of the call for proposals at http://www. bmbf.de and http://www.vr.se.

An English translation of the complete BMBF call is available at http://www.rontgen-angstrom.eu.

## FACTS ABOUT PETRA III EXTENSION

New experimental halls	2
New beamlines	10
Project cost	ca. 85 million Euro
First beam	expected in fall 2015



Existing PETRA III hall on DESY campus in March 2015 © Britta von Heintze

## **EDITORIAL**

2015 promises to turn into yet another productive year for everyone involved in the Röntgen-Ångström-Cluster. A new call for RÅC research proposals has been launched by the Swedish and German governments. While keeping you posted on progress made by the previous recipients of RÅC funding (please read two progress reports below), we look forward to introducing new projects in the near future. Please spread the word and keep your exciting ideas coming. Inspiration can be drawn from site at DESY where construction work is ongoing. On top of potentially providing new incentives, the numerous building sites on the Hamburg campus, featured exclusively in this issue, can also be seen as reflecting the diverse research undertaken by RÅC scientists across the Baltic sea. As new research facilities emerge at DESY, new scientific results and initiatives come to light.

The editorial team undertook an expedition across DESY's PETRA III construction site and managed to capture the impressive works in images and text. Meanwhile, scientists in other parts of Germany and Sweden have been busy contributing their bit to further the cause of the Röntgen-Ångström-Cluster.

Also in this issue: Martin Hällberg and Hans Hertz, two Swedish recipients of RÅC-funding, update us about their doings and findings while Andreas Schreyer shares detailed info on MATRAC II, a new version of the successful MATRAC I with a slightly different focus. The German-Swedish school will kick off in 2016.

Another newcomer is the RACIRI Summer School, as this already well established programme will take place in Germany for the first time later this year. Furtherdown, the organisors reveal a world renowned key note speaker. Last but not least, check out "the OTHER news" for yet another potentially first-ever event of its kind to take place in Hamburg.

The editors

## **NEWS**

### PETRA III EXTENSION: WATCHING WORK IN PROGRESS



A hustle and bustle is going on on DESY campus in Hamburg these days. Currently, there are no fewer than eight projects under construction or being planned. Among them, the extension of world's brightest synchrotron radiation source PETRA III is in full development. On an area of 6000 square metres, two new experimental halls are being raised north and east of the existing large "Max von Laue" hall, with an additional 1400 square metres providing office and laboratory space for scientists. The experimental halls will host ten new beamlines which are designed in close cooperation with the photon science user community.



Civil engineering for the PETRA III extension project started in December 2013 to expand the brilliant X-ray source's research capabilities and to meet the increasing user demand. Wolfgang Caliebe, leader of work package "Time-resolved and Bio X-Ray Absorption Spectroscopy", kindly took us on a photo tour to the PETRA III construction sites where we could catch a glimpse of work in progress.



The new PETRA III north hall is built adjacent to FLASH II, the extension of DESY's free-electron laser FLASH. Beside the building with its characteristic orange lining, an earth wall functions as additional protection from X-rays since the PET-RA III tunnel runs above ground in this area. The two facilities are going to be connected in order to encourage communication between the scientists.

### NEWS



Interior view of the north hall in March 2015, showing the still empty experimental floor where the new beamlines and instruments will be located. The PETRA III tunnel is located above ground beneath the massive concrete on the right. The doorways on the left are meant for future laboratories (ground floor) und rooms for personnel (upper floor). Researchers, especially chemists, biologists and geologists, will get the chance to use new beamlines, including time-resolved X-ray absorption spectroscopy, high-energy as well as high-pressure materials science and time-resolved luminiscence spectroscopy. "When we started planning five years ago, detectors were not as advanced as they are today. Now we can install even better and more efficient experimental stations than we originally assumed", Wolfgang Caliebe reveals.



Looking into the east hall in March 2015. Here, the ring tunnel lies completely underground, i.e. the experimental floor is in the "basement". Heavy concrete-shielding hutches are already completed to host essential X-ray optics like mirror and slit systems, refractive lenses and monochromators. The east hall will contain five undulator beamlines for high-energy materials science and X-ray diffraction, X-ray nano-spectroscopy and chemical crystallography. One of these new beamlines is funded by Sweden. It will be operated by DESY in collaboration with a consortium of Swedish universities, namely the Royal Institute of Technology in Stockholm and Linköping University. Furthermore, in the framework of German-Swedish cooperation, the Röntgen-Ångström-Cluster develops and provides new instrumentation for the experimental stations.



Some techniques and experiments such as X-ray absorption spectroscopy and chemical crystallography (the photo shows a so-called "Kappa diffractometer") are not yet available at PETRA III, but had been very successfully performed at DESY's former storage ring DORIS III. With the PETRA III extension, users will find a new scientific home for these techniques. What is more, researchers will profit from the excellent beam conditions at PETRA III: At several experimental stations, the beam will be up to one hundred times more intense compared to DORIS III, which reduces data collection times and improves data quality.

## PROJECTS

### SOMETHING TRULY UNIQUE



Martin Hällberg, Senior Researcher in the Department of Cell and Molecular Biology at Karolinska Institute in Stockholm and recipient of funding awarded in the context of the Röntgen-Ångström-Cluster, writes about his efforts of setting up a research group associated with the "Centre for Structural Systems Biology" (CSSB), a

facility in the making in Hamburg, and about the results the group has achieved up to this day.

In late 2011, I obtained a grant from the Swedish Research Council related to its RAC programme to set up a junior research group at the DESY campus in Hamburg. This group is associated with the newly formed Centre for Structural Systems Biology (CSSB). The CSSB is an initiative of nine research partners aimed at building up a world-class center for systems and structural biology on DESY campus. Financed by a €52-million grant from the Federal Republic of Germany, the City of Hamburg, Lower Saxony and Schleswig-Holstein, the CSSB is constructing a 13,500 square meter research building beside the PETRA III experimental hall. The building is planned to host a range of infrastructures for biophysical characterisation and crystallisation as well as two state-of-the-art cryoelectron microscopes and ultrahigh resolution visual light microscopes. The CSSB facility will support structural biology research on the whole cellular scale, which is something truly unique.

The CSSB building is expected to be finished in early 2017. While waiting for the new building, we have been allocated space in the 25b building at the DESY campus beside the European Molecular Biology Laboratory (EMBL). Here, we have built up a full-fledged structural biology laboratory. For advanced biophysical characterisation, we are using the Sample Preparation and Characterisation facility just across the road by the EMBL beamlines for macromolecular crystallography and biological small-angle scattering. In the initiation phase of the project we solved and published the structure of a maturation factor for mitochondrial ribosome in collaboration with Professor Nils-Göran Larsson's Group at the Max-Planck Institute for the Biology of Ageing.<sup>1</sup> During the following establishing phase in Hamburg, we have crystallized and solved the structure of two very important proteins in mitochondrial RNA processing, and these are currently submitted for publication. Furthermore, in collaboration with Professor Claes Gustafsson's group at Gothenburg University, we have published two exciting biochemical results on mitochondrial transcription.<sup>2, 3</sup> My current RÅC-financed group associated with the CSSB in Hamburg consists of two post-docs and two PhD students, a group size we aim to keep during the coming years. We are, of course, very much looking forward to moving into the new CSSB building in 2017 with its unique mixture of techniques aimed at elucidating biology on all cellular scales. This building is near some fantastic large-scale facilities such as the PETRA III and the European X-FEL. This situation brings to mind the words of a real estate broker: "Location, location, location".

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[3] TEFM is a potent stimulator of mitochondrial transcription elongation in vitro. Posse
V, Shahzad S, Falkenberg M, Hällberg BM, Gustafsson CM. (2015) Nucleic Acids Res. 43, 2615-2624



CSSB construction site on DESY campus in March 2015 © Britta von Heintze

## **ANNOUNCEMENTS**



## SECOND SWEDISH-GERMAN WORKSHOP ON X-RAY OPTICS

The second Swedish-German workshop on X-Ray optics took place on 28-30 April 2015 at the Helmholtz-Zentrum Berlin, as reciprocal meeting to the first workshop held in March 2012 in Åhus Strand, Sweden. The aim

of the event was to maintain a long-term relationship and close cooperation between Germany and Sweden and to therefore bring together scientists and engineers of research institutes from both countries.

This year the workshop covered topics such as the optical system design for ultra-high time and spectral resolution, optical technology and metrology, and FEL/XFEL optics. It also focused on future projects for new facilities like BESSY–VSR, the PETRA III extension and MAX IV, and offered the opportunity to establish international collaborations as well as joint research and development programs in the field of advanced X-ray optics for future X-ray sources. The International Advisory and Program Committee (Alexei Erko, HZB; Frank Siewert, HZB; Franz Hennies, MAX IV; Yngve Cerenius, MAX IV; Jesper Anderson, MAX IV; Rolf Follath, PSI) expected approximately 40 participants and slightly more than 30 talks. Financial support was provided by the BMBF (Röntgen-Ångström-Cluster program) and Helmholtz Zentrum Berlin.

Photo: Alexei Erko, Director of Institute for Nanometre Optics and Technology, HZB

## PROJECTS

### PRACTICALS IN NEUTRON RESEARCH



In this exclusive interview, Professor Andreas Schreyer from Helmholtz-Zentrum Geesthacht talks about the new initiative MATRAC II.

# What were the reasons behind launching the new initiative "MATRAC II" ?

There are two reasons for launching "MA-TRAC II". Firstly, until 2010 the Helmholtz-Zentrum Geesthacht, Centre for Materials and Coastal Research, had its own research reactor (editor's note: the research reactor FRG-1 was in use between 1958 and 2010 and was one of the first of its kind in Germany). In practice, switching off the FRG-1 meant that the Helmholtz-Zentrum was no longer in a position to offer internships and practical training in the area of neutron research. There was a general consensus that we had to find ways to compensate for this deficit.

Secondly, in the context of the Röntgen-Ångström-Cluster, Sweden expressed a keen interest in creating opportunities for young scientists to experience neutron research and receive some practical training, similar to the way this is being planned by the European Spallation Source (ESS) in Lund.

These two reasons led us to act and consequently establish MATRAC II, not as a successor of its successful forerunner MA-TRAC I, but as a complementary school dedicated to young scientists in order to provide them with the means of experiencing neutron research and undergo some practical training under the supervision of experts.

### Could you explain the concept of MATRAC II? How does it differ from its predecessor MATRAC I?

MATRAC I started in 2005 and takes place every two years, very successfully. Up to 60 students participate in the five-dayevent in Hamburg/Geesthacht and they do that with a lot of enthusiasm. But: MATRAC I only offers practical training in the area of synchrotron radiation at DESY. MATRAC II, on the other hand, offers such practicals in the area of neutron research. The latter takes place in Garching (editor's note: at the Heinz Maier-Leibnitz Zentrum (MLZ), operating the research reactor FRM II, which is currently the most powerful source of its kind in Germany). In terms of structure, both schools are very similar. There are three days worth of lectures focusing on the current state of the art and the most pressing questions in sciences. The rest of the time is devoted to practical training. The students are divided in smaller groups and get the opportunity to apply their theoretical knowledge in practice and use the research facilities.

### Who is the target group?

The schools are aimed at an international audience on the level of master and PhD students as well as young Postdocs. In the past, the number of participants from Germany amounted to roughly two thirds, the other third joined from abroad, mostly from other European countries. In the future, with the background of ESS being built in Sweden, we'd like to raise the number of applicants from Sweden.

Students apply with their CV and information about their work so far. We get a lot more applicants than we have places available so our selection is largely based on the emphasis of the work of each student. Thematically, it has to match the content of the MATRAC schools, i.e. materials science.

### Is there financial support?

Normally, within the RÅC each country is in charge of paying its own bill. The Swedish Research Council, for example, is responsible for the Swedish participants. The Federal Ministry of Research and Education takes charge of the German students. In addition students from EU countries other than Germany also qualify for EU funding, typically in form of contributions to the travel costs.

### When will MATRAC I start?

MATRAC I takes place in uneven years, MATRAC II in even years. This being 2015, it's MATRAC I's turn this year. The school is scheduled for September 21 to 25. We're currently in the process of completing the programme. All information will be available at http://www.hzg.de/matrac.

## **The OTHER News**

#### HAMBURG 2024: ON THE BRINK OF ATHLETIC EXCELLENCE?

On your marks, get set, go: Hamburg is set to bid for the 2024 Summer Olympic Games, beating Berlin as the German choice as was announced by the German Olympic Committee in March. That makes it the only German contender and the first possible German Olympic city since Munich 1972 and Berlin 1936. Hamburg, home to DESY and the European XFEL, aims high. Germany's second largest city wants to show the world that hosting Olympic Games is not about investing billions in state of the art venues that will be left to ruin once the Games are finished. Hamburg's concept, titled "Games of the short ways in the heart of the city", is about sustainability. Still, Hamburg is up against fierce competition from around the globe: Boston, Rome, possibly Paris, Istanbul, Doha and Baku. The host will be chosen in an International Olympic Committee members vote in Peru in 2017. Before Hamburg starts its official campaign, the city needs to find out if it will get the citizen's support. Do the people of Hamburg want the Olympic Summer Games 2024 featuring athletic excellence between Alster and Elbe? German officials take this aspect seriously, bearing in mind that Munich failed to win the support of the local population in a referendum on hosting the Winter Games 2022. Hosting Olympic Games is a project for the entire nation. Home Secretary Thomas de Maizière puts it like this: "For the sake of the Olympics, we all are Hamburgians from now."

Although a far cry from the Olympic Games, the Röntgen-Angström-Cluster may set a prime example here: Reaching out across borders to work together in the interest of one goal produces excellent results. In the case of the RÅC, it's Materials Sciences.

### PROJECTS

### PROGRESS REPORT: RESOLUTION IN BIOLOGICAL 3D SOFT X-RAY NANO IMAGING



Hans Hertz, Professor of Applied Physics at the KTH Royal Institute of Technology in Stockholm, gives an update on his work funded and undertaken in the context of the Röntgen-Ångström-Cluster.

The project goals were summarised by the abstract in the original proposal: "The primary goal of the present proposal is to de-

termine the ultimate achievable resolution in three-dimensional (3D) soft x-ray cryo tomography of intact cells. In addition to its biological relevance, the projects address a classical imaging problem: to obtain high spatial resolution with sufficient contrast in intact thick bio objects like cells. The project relies on combining advanced theoretical modeling of the imaging process with experiments at the HZB synchrotron-based x-ray microscope. The work primarily involves computational physics, optics, illumination, contrast, reconstruction and noise in partially coherent and dose-limited systems."

We have now successfully finished the computational parts of the project. Here we have developed a full 3D wave-propagation model that better describes the image formation process of zone-plate based x-ray microscopes.<sup>1</sup> In these microscopes the studied object is typically larger than the depth of focus (DOF) and the sample illumination is often partially coherent. The model is compared with previous simulation methods as well as with experiments at the HZB transmission x-ray microscope and the results show that our model predicts the image formation of transmission soft x-ray microscopes more accurately than previous models. Based on this model we then designed an improved tomographic reconstruction method to achieve high resolution in the full sample when the DOF is short compared to the sample thickness.<sup>2</sup> The method relies on the back-projection of focus-stacked image data from x-ray microscopy. We demonstrated the method on theoretical and experimental data. All work has been done in collaboration with the Schneider group at HZB Berlin. The next steps will be to implement the methods for laboratory x-ray microscopy. This is an involved task since simulations show that a certain degree partial coherence is advisable which will reduce our photon flux. Work is presently performed to increase the photon flux from our laser-plasma source further.<sup>3</sup>

M. Selin, E. Fogelqvist, A. Holmberg, P. Guttmann, U. Vogt, and H. M. Hertz, "3D Simulation of the Image Formation in Soft X-Ray Microscopes", Opt. Expr. 22, 30756 (2014).
M. Selin, E. Fogelqvist, S. Werner, and H. M. Hertz, "Tomographic reconstruction in soft x-ray microscopy using focus-stack back projection", subm. Opt. Lett. [3] D. H. Martz, M. Selin, O. von Hofsten, E. Fogelqvist, A. Holmberg. U. Vogt, H. Legall, G. Blobel, C. Seim, H. Stiel, and H. M. Hertz, "High-brightness liquid-jet laser-plasma source for waterwindow microscopy", Opt Lett. 37, 4425 (2012)

### ANNOUNCEMENTS

### **RACIRI SUMMER SCHOOL 2015 IN GERMANY**

This year, the RACIRI Summer School will be held in Germany for the first time. One of the highlights of the seven-day event is undoubtedly the keynote lecture held by 2009 Nobel Prize Winner of Chemistry, Ada Yonath from Israel, the first woman in 45 years to win this most prestigious prize.

The appointment of Ada Yonath as the keynote speaker is especially appropriate as the RACIRI Summer School is aimed at the next generation of materials scientists. The 76-year-old structural biologist will share the wealth of her experiences with the future researchers who can expect to take away precious insights into a life devoted to sciences. The school will address PhD students, master (diploma) students and young Postdocs coming mainly from institutions of the three partnering countries.

How to apply: Spaces are limited. RACIRI 2015 holds up to 80 places in total for applicants from universities and scientific institutes. Admission is based on national calls in the partner countries Russia, Germany and Sweden and granted through a nomination process according to scientific excellence. Each country will organize the calls and the selection process autonomously. The selected scholars will receive all necessary funding for travel, accommodation and food.

When? 22 – 29 August 2015 Where? Rügen Island, Cliff Hotel Rügen For more info visit: http://www.raciri.org

Launched in 2013, the RACIRI initiative is based on two bilateral cooperation platforms, the German-Swedish Röntgen-Ångström-Cluster RÅC (http://www.rontgen-angstrom.eu) and the German-Russian loffe-Röntgen Institute IRI (www.iofferoentgen.org). RACIRI enjoys an excellent reputation and has already established itself as an institution. All RACIRI Summer Schools are dedicated to the overall theme of "Advanced Materials Design at X-ray and Neutron Facilities". The structure of the summer school provides a stimulating learning environment with sufficient time for social and cultural activities among the students. Internationally renowned scientists and experts from the relevant fields are invited as lecturers and tutors to engage in a close dialogue between the generations. The RACIRI Summer Schools are financed by the Russian Foundation for Basic Research (RFBR) and the NRC "Kurchatov Institute", the Federal Ministry of Education and Research (BMBF) and the Swedish Research Council "Vetenskapsrådet".

### IMPRINT

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