



No. II/15 - 30 June 2015

# PSI photon, neutron and muon user facilities newsletter

## Editorial



Oliver Bunk

Dear colleagues,

Macromolecular crystallography (MX) has sometimes been perceived as a technique that has been so highly optimized that it has reached a static regime: MX produces structures in the Protein Data Bank (**PDB**)

<http://www.rcsb.org/pdb/home/home.do> ,

high profile papers and Nobel prizes, but does not develop any further from a method and instrumentation point of view. An important contribution to a more dynamic perception of MX has been spurred by X-ray free electron lasers (XFELs). Already, the first pioneering work exploring single molecule diffraction in a 'diffract before destroy' approach pointed out that the flux is simply not enough for it to work as single shot technique. But it sparked the advent of serial crystallography, with its promise of providing diffraction data at a resolution that is not limited by radiation damage.

These developments promoted work at storage ring sources on new sample delivery methods and on merging data recorded for many small crystals. In turn, the analysis of XFEL data is benefitting from the experience collected at conventional sources. This setting diversifies even further with long term projects coming to fruition. The next detector generation EIGER will benefit data quality and enable a closer look on recent findings of a delayed onset of radiation damage in studies at room tempera-

## New calls for proposals

### **SLS: non-PX beamlines**

deadline: September 15, 2015

### **SLS: PX-beamlines**

deadline: October 15, 2015

### **more information**

<http://www.psi.ch/sls/calls>

### **SINQ**

deadline: November 15, 2015

### **more information**

<http://www.psi.ch/sinq/call-for-proposals>

### **SμS**

deadline: December 2015

### **more information**

<http://www.psi.ch/smuscalls>

An **overview** about all proposal submission deadlines of the PSI facilities can be obtained **here** <http://www.psi.ch/useroffice/proposal-deadlines> .

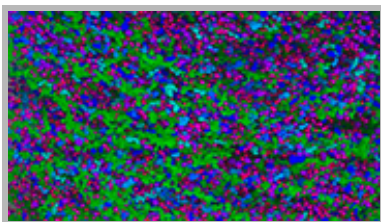
ture. The **PRIGo** <<http://dx.doi.org/10.1107/S1600577515005354>> multi-axis goniometer, developed in-house as well, and its successor SmarGon are significantly extending the range of molecules accessible to phasing based on the weak anomalous scattering from sulfur atoms in particular. Advances in single-particle imaging at cryo electron microscopes helped drawing the line between the core applications of each of those techniques. New machines and upgrades of existing storage rings make it possible to obtain brilliant micro-focus X-ray beams of low divergence.

All in all, the field of MX is remarkably dynamic. XFELs and storage rings do not just complement each other. The ongoing developments stimulate each other and benefit the whole field. At institutes like PSI with **Swiss-FEL** <<http://www.psi.ch/swissfel/>> and **SLS** <<http://www.psi.ch/sls>> on the same site, this feedback loop can be direct and efficient. The close link to the synchrotron user community built up over the past 15 years helps channeling these developments in directions useful for state-of-the-art scientific applications. The future at storage rings and XFELs is bright and dynamic, and I am looking forward to shaping part of it together with you.

Oliver Bunk, Head of the Laboratory for Macromolecules and Bioimaging '**LSB**' <<http://www.psi.ch/lb/>>, Department SYN, PSI

## Research highlights

### SLS - Materials Science: Extremely detailed 3D images



#### From Inside an Eggshell

**Manuel Guizar-Sicairos et al, Optica 2, 259--266 (2015), DOI:10.1364/OPTI-**

## Facility news

### SLS: Acknowledgement of SLS facilities and European Grants

Any publication resulting from a SLS beamtime project with scientific and technical contribution from SLS scientist(s) should include these person(s) as co-author(s). In case the SLS support of the research team was limited to technical assistance the authors must mention at least Paul Scherrer Institut, SLS, the instrument and the beamline/station support in the acknowledgement, for example in the form: "We acknowledge the Paul Scherrer Institut, Villigen, Switzerland for provision of synchrotron radiation beamtime at beamline ### of the SLS and would like to thank xyz for assistance."

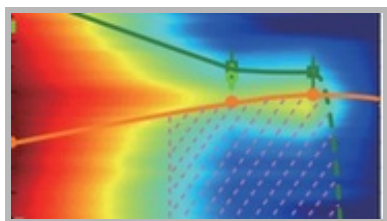
All publications resulting from SLS experiments, which were funded within one of the EU Access programs should contain the following acknowledgement statement: "The research leading to these results has received funding from the European Community's Seventh Framework Programme (FP7/2007-2013)

**CA.2.000259** <<http://dx.doi.org/10.1364/OPTICA.2.000259>>

Tiny voids inside eggshells supply the materials that stimulate and control the shell's growth. Using a novel imaging technique, researchers from the Paul Scherrer Institute (PSI), ETH Zurich and the Dutch FOM Institute AMOLF have succeeded in imaging these voids in 3D for the first time. In doing so, they lift an old limitation of tomographic images and hope that one day medicine will also benefit from their method.

The new technique could be used to image sections of an object in high resolution more quickly, without burdening the object's surroundings unnecessarily strongly with radiation. This could also make the method interesting for medical applications. Computer images of part of an organ would be conceivable, for instance, without having to irradiate the patient's whole body intensely. The radiation could therefore be focused on the part of an organ that one wants to study, largely sparing the surrounding tissue. In terms of hardware, no major obstacles should stand in the way of the new technique as it does not depend on x-ray light from a large research facility like the SLS.

**Read the full story** <<http://www.psi.ch/media/from-inside-an-eggshell>>

**SINQ - Phase transitions and superconductivity**

<<http://www.psi.ch/num/2015#hu>>

## Structural and Magnetic Phase Transitions near Optimal Superconductivity in $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

**D. Hu et al, Physical Review Letters 114, 157002 (2015),**

under grant agreement n. °312284 for CALIPSO, n. °283570 for BioStruct-X or n. °262348 for ESMI." The SLS management thanks very much for the cooperation in this matter.

**SINQ: More space for new sample environment on SANS-II**

The small-angle neutron scattering instrument SANS-II was modified to allow a wider range of sample environments. The collimation and detector noses were redesigned using non-magnetic materials and optimised for reduced background. The adapted beamstop size provides more flexibility when choosing between higher neutron counts and larger momentum transfer range.

An immediate consequence of these improvements is the possibility of using on SANS-II a very large cryomagnet, MA7 with its magnetic field up to 6.8 T. A big advantage of MA7 is the relatively large experimental space (48 mm of diameter) available for sample, sample holder, and auxiliary equipment in the sample area.

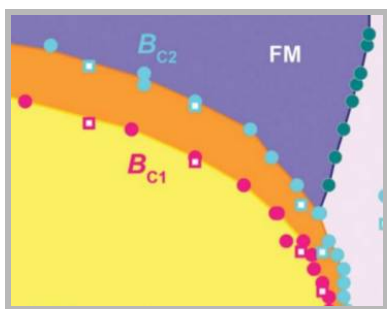
**DOI: 10.1103/PhysRevLett.114.157002** <<http://dx.doi.org/10.1103/PhysRevLett.114.157002>>

[doi.org/10.1103/PhysRevLett.114.157002](http://dx.doi.org/10.1103/PhysRevLett.114.157002)

We use nuclear magnetic resonance (NMR), high-resolution x-ray, and neutron scattering studies to study structural and magnetic phase transitions in phosphorus-doped  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ . Previous transport, NMR, specific heat, and magnetic penetration depth measurements have provided compelling evidence for the presence of a quantum critical point (QCP) near optimal superconductivity at  $x=0.3$ . However, we show that the tetragonal-to-orthorhombic structural ( $T_S$ ) and paramagnetic to antiferromagnetic (AF,  $T_N$ ) transitions in  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$  are always coupled and approach  $T_N \approx T_S \geq T_C$  ( $\approx 29$  K) for  $x=0.29$  before vanishing abruptly for  $x \geq 0.3$ . These results suggest that AF order in  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$  disappears in a weakly first-order fashion near optimal superconductivity, much like the electron-doped iron pnictides with an avoided QCP.

**Read the full story** <<http://www.psi.ch/num/2015#hu>>

### **$\mu$ S and SINQ - Material Science – Using metamagnets for broadband electromagnetic filtering**



<<http://www.psi.ch/num/2015#pregelj>>

### **Controllable Broadband Absorption in the Mixed Phase of Metamagnets**

**M. Pregelj et al, Advanced Functional Materials, adv. online publ. (2015), DOI: 10.1002/adfm.201500702**

<<http://dx.doi.org/10.1002/adfm.201500702>>

Materials with broad absorption bands are highly desirable for electromagnetic filtering and processing ap-

### **$\mu$ S: New developments at the LEM apparatus**

In the past, the accessible field range for longitudinal and transverse field  $\mu$ SR studies on the LEM spectrometer was restricted due to the formation of Penning traps for ions in the sample region where the electric field of the last focusing lens and the experimental magnetic field overlap. With the help of a new high voltage power supply and the development of an "on/off" measurement mode, the high voltage of the electrostatic lens can now be pulsed which effectively evacuates the Penning traps periodically. This allows the use of magnetic fields in the whole available field range up to 3000 G with a duty cycle of 90% while maintaining a narrow beamspot. In addition the new "on/off" mode can be used for  $\mu$ SR experiments with external stimuli like electric fields, radio frequency or light.

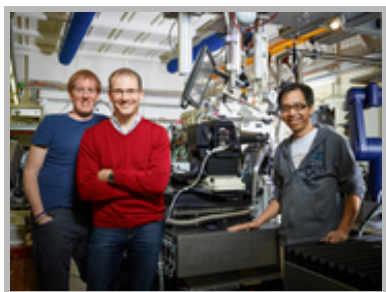
### **SwissFEL: PSI-DESY Collaboration Delivers First Photonics Component for SwissFEL**

The Photon Beam Intensity Gas (PBIG) monitor arrived at PSI at the end of May, and

plications, especially if the absorption can be externally controlled. Here, a new class of broadband-absorption materials is introduced. Namely, layered metamagnets exhibit an electromagnetic excitation continuum in the magnetic-field-induced mixed ferro- and antiferromagnetic phase. Employing a series of complementary experimental techniques involving neutron scattering, muon spin relaxation, specific heat, ac and dc magnetization measurements, and electron magnetic resonance, a detailed magnetic phase diagram of  $\text{Cu}_3\text{Bi}(\text{SeO}_3)_2\text{O}_2\text{Br}$  is determined and it is found that the excitations in the mixed phase extend over at least ten decades of frequency. The results, which reveal a new dynamical aspect of the mixed phase in metamagnets, open up a novel approach to controllable microwave filtering.

**Read the full story** <<http://www.psi.ch/num/2015#pregelj>>

### SwissFEL - Decoding biomolecules at SwissFEL and SLS



<[http://www.psi.ch/media/to-](http://www.psi.ch/media/together_not_alone)

gether\_not\_alone>

## Together, not alone

Proteins are a coveted but stubborn research object. A method developed for x-ray free-electron lasers and PSI's future SwissFEL should now help researchers to make good headway in this field. It involves x-raying many small, identical protein samples consecutively at short intervals, thereby avoiding the main problem that protein research has faced thus far: producing samples in a sufficient size.

will be one of the first photonics components to be installed in the new SwissFEL facility. The device has been developed and adapted to fit the SwissFEL parameters in a PSI-DESY collaboration over the course of two years. The gas-based detectors, designated as the Photon Beam Intensity Gas (PBIG) monitor and the Photon Beam Position Gas (PBPG) monitor will be the first components to see the photon beam created by the SwissFEL, and will be the main components that users and operators will use to optimize the operations of the machine and to better understand the data collected. The photon beam position and intensity monitors detect the position and intensity of the FEL beam by counting the number of ions created in a pre-calibrated gas chamber through the photoionization process, and looking at the differences in a split electrode to find the position of the beam, **read more**

<<http://www.psi.ch/swissfel/highlights>> .



**Read the full story** <[http://www.psi.ch/media/together\\_not-alone](http://www.psi.ch/media/together_not-alone)>

**Watch a short video on serial crystallography on YouTube** <<https://www.youtube.com/watch?t=37&v=ZqJaUEb78hc>>

## Users Association

### JUSAP - The Joint Users Association



<<http://www.psi.ch/userof->

[fice/users-association](http://www.psi.ch/userof-fice/users-association)>

Sarah Dunsiger

The 8th Annual Meeting of the European Synchrotron User Organization (ESUO) took place at the Helmholtz Zentrum Berlin (HZB) on April 27-28, 2015. The minutes of the meeting are **accessible here** <<http://www.esuo.org/?node=8thESUOMeeting>>. The three year **CALIPSO project** <<http://www.calipso.wayforlight.eu>> funded by the European Commission under the FP7-Infrastructures programme ended on May 31, 2015. However, thanks to recent lobbying initiatives, the topic "Synchrotron radiation sources and Free Electron Lasers" is now included in the draft of the Horizon 2020 Research Infrastructures Work Programme 2016-2017. In the new work programme a call is expected for both a synchrotron/FEL (CALIPSO+) as well

## Upcoming events

### ICM2015: 20th International Conference on Magnetism

<<http://www.icm2015.org>>

July 5-10, 2015, Barcelona, Spain

### SRI2015: 12th International Conference on Synchrotron Radiation Instrumentation

<<http://www.bnl.gov/sri2015/>>

July 6-10, 2015, New York, USA

### SynLight 2015: Recent Developments in Synchrotron Radiation

<<http://pages.cnpem.br/synclight2015/>>

July 13-24, 2015, Campinas, Sao Paulo, Brazil

### AOCNS-2015: 2nd Asia Oceania Conference on Neutron Scattering

<<http://www.aocns-2015.com>>

July 19-23, 2015, Sydney, Australia

### COR S.O. 2015: New Physics due to spin-orbit coupling in correlated electron systems

<<http://corso2015.sciencesconf.org>>

August 4-14, 2015, Cargese (Corse), France

### PSI Summer School on Condensed Matter Research

as for a neutron/muon I3 (NMI3+) access programme. The deadline for both proposals is expected to be March 30, 2016.

There will be an estimated gap of about 18 months without transnational access funds for synchrotron and FEL users. However, European large research facilities have agreed to financially support both ESUO and the **wayforlight tool** <<http://www.wayforlight.eu>> through a post-CALIPSO bridging agreement, to assure the continuation of their activities.

The close cooperation between large research facilities and their user communities is essential. To that end, following an incident at PSI where a user removed an activated sample from one of the facilities without a radiation check, JUSAP would like to remind users it is very important to observe the **PSI safety regulations** <<http://www.psi.ch/useroffice/safety-at-psi>> . To avoid the necessity of making those regulations more stringent in future, it is essential to maintain the current safety culture, where PSI staff and management have confidence in the user community.

Yours sincerely,

Sarah Dunsiger (JUSAP committee chair)

**2015** <<http://www.psi.ch/summerschool>>

**August 15-21, 2015, Zuoz, Switzerland**

**M2S 2015: 11th International Conference on Materials and Mechanisms of Superconductivity**

<<http://www.m2s-2015.ch>>

August 23-28, 2015, Geneva, Switzerland

**ECNS2015: VI European Conference on Neutron Scattering** <<http://www.ecns2015.eu>>

August 30 - September 4, 2015, Zaragoza, Spain

**Joint annual meeting of the Swiss and the Austrian Physical Society**

<<http://www.sps.ch>>

September 1-4, 2015, Vienna, Austria

**SRPS6: VI International Conference of Synchrotron Radiation in Polymer Science** <<http://srps6.com>>

September 7-10, 2015, Madrid, Spain

**19th JCNS Laboratory Course Neutron Scattering**

<<http://www.neutronlab.de>>

September 7-18, 2015, Jülich and Garching, Germany

**SAS2015: 16th International**

**conference on Small-Angle Scattering** <<http://www.-cac.us.edu.pl>>

cac.us.edu.pl&gt;

September 13-18, 2015,  
Berlin, Germany**AUNIRA: Training Workshop on Advanced Use of Neutron Imaging for Research and Applications** <<https://indico.psi.ch/conferenceDisplay.py?confId=3679>>

co.psi.ch/conferenceDisplay.py?

confId=3679&gt;

**September 28 - October 2, 2015, PSI Villigen, Switzerland****more events** <<http://www.psi.ch/useroffice/conference-calendar>>

si.ch/useroffice/conference-calendar&gt;

## Current Openings

**Job opportunities at PSI**<<http://www.psi.ch/en/pa/offenstellen/>>

## Announcements

### PSI Summer School 2015

The 2015 (14th) PSI summer school on condensed matter research will again be organized at the Lyceum Alpinum in Zuoz/CH from **August 15-21, 2015**. The PSI summer schools aim to train young researchers in the methods being used at large research facilities such as neutron and muon sources or synchrotron photon sources. International experts and PSI staff members will introduce and deepen your knowledge not only on those methods but also on the phenomena, which are presently at the forefront of modern solid state research.



Following the school a practical training is offered at PSI (August 22-23). It will allow a limited number of participants to get hands-on experience with state-of-the-art instrumentation using photons, neutrons, and muons. The online application will open early 2015. Please visit the **school's homepage** <<http://indico.psi.ch/conferenceDisplay.py?confId=3407>> for more information.

### In Situ Serial Crystallography Workshop at the SLS

The Macromolecular Crystallography group at SLS headed by Dr. Meitian Wang is organizing a three days **workshop on in situ serial crystallography** <<http://indico.psi.ch/event/issx>> between November 17 and 19, 2015. It will be dedicated to the presentation of a novel method facilitating the structure determination of membrane proteins, which are highly important pharmaceutical targets but are difficult to handle using "classical" crystallographic tools. Designed for 20 PhD students, postdocs and young scientists from both academia and industry, the workshop will consist of introductory lectures, followed by hands-on practicals on in meso or lipidic cubic phase (LCP) crystallization, on in situ serial crystallography data collection using a micro-sized beam and on data processing. The method, which will be demonstrated at the SLS, will be applicable at the future SwissFEL.

### Proprietary research

A certain fraction of the beamtime at PSI research facilities is reserved for proprietary use. This is handled by the **PSI Technology Transfer** <<http://www.psi.ch/industry/technology-transfer>> . The following **directory** <<http://www.psi.ch/industry/expertise>> lists services on offer by these facilities. For the SLS beam lines industrial use is facilitated by the SLS Technology Transfer AG. If you are not an expert in a particular technique or you are unsure which technique is best suited for your application(s), please contact us via the email address published on the **SLS TT homepage** <<http://www.psi.ch/sls-techno-trans-ag/sls-techno-trans-ag>> .

### Imprint

PSI Facility News addresses the users of the PSI large facilities and appears quarterly in English. Any feedback is highly welcome! **More information.** <<http://www.psi.ch/imprint>>

**Contact:** PSI User Office, Phone: +41-56-310-4666, Email: [useroffice@psi.ch](mailto:useroffice@psi.ch)