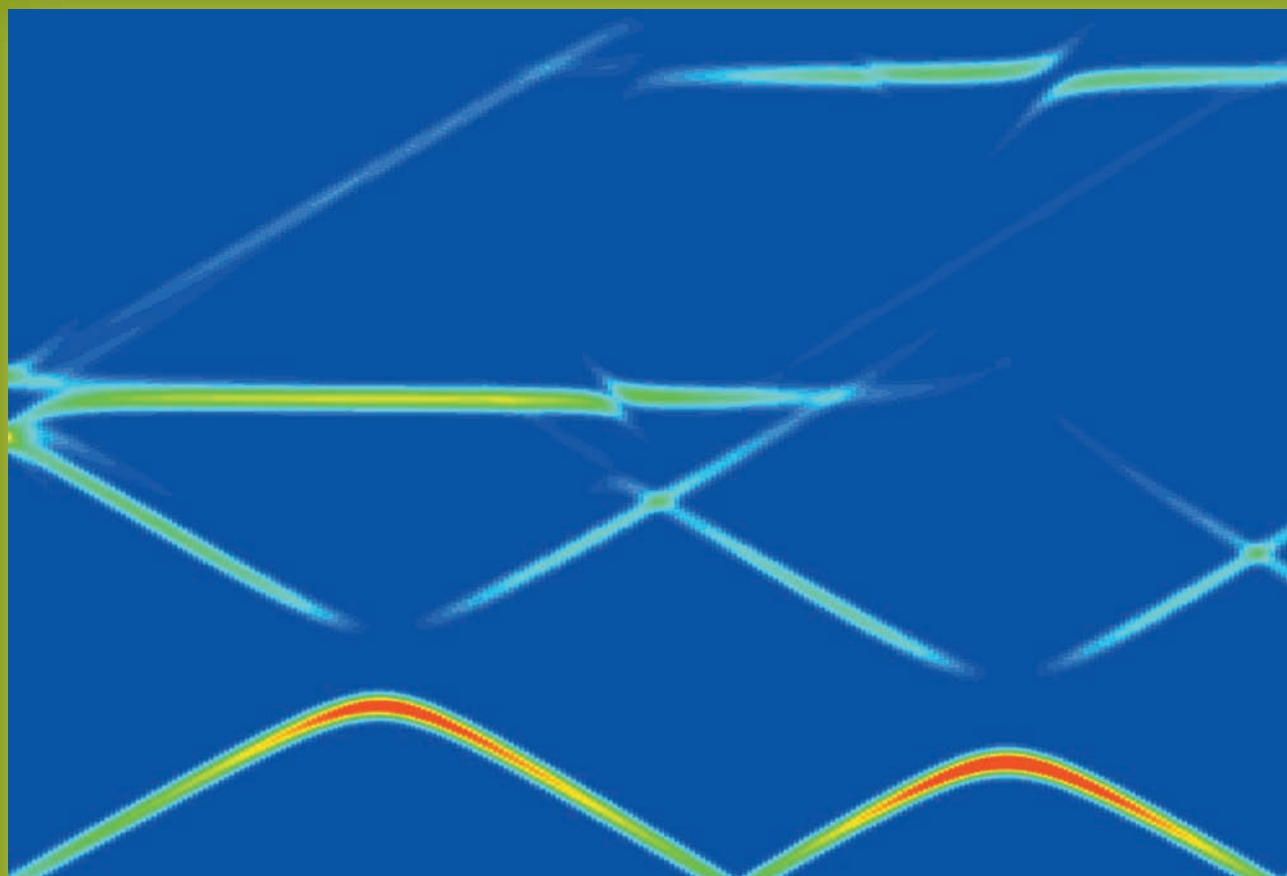


# NOTIZIARIO

## Neutroni e Luce di Sincrotrone



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Scientific Reviews

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# SUMMARY

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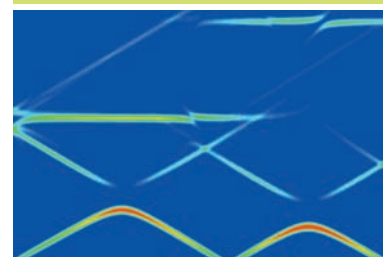
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J. Bellingham (NMI3)  
M. Bertolo (I3-IA-SFS)  
A.E. Ekkebus (SNS)

#### ON LINE VERSION

V. Buttarò

#### CONTRIBUTORS TO THIS ISSUE

M. Capellas, M. Krisch, H. Schober

#### PREVIOUS ISSUES AND EDITORIAL INFORMATION

Pina Casella  
Università degli Studi di Roma Tor Vergata  
Presidenza Facoltà di Scienze M.F.N.  
Via della Ricerca Scientifica, 1  
00133 Roma  
Tel: +39 06 72594304  
E-mail: nlns@roma2.infn.it

#### GRAPHIC AND PRINTING

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Via Fabrizio Lusino 73  
00174 Roma

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**Cover photo.** INS cross section of Cr<sub>7</sub>Ni as a function of magnetic field and energy transfer.



# Neutrons, Airlines and the ESS

**H. Schober**

*Institut Laue Langevin, Grenoble, France*

At first sight airlines have little in common with neutron facilities. If one, however, takes a closer look then one discovers that the business they do shares many similarities. Like aviation infrastructure neutron infrastructure is expensive and delocalized. It has to cater to the needs of a geographically spread-out clientele with a broad bandwidth of specific needs. Being expensive and anchored in an internationally competitive environment both infrastructures have to be used to their best to survive.

It is thus somewhat surprising that the business plans developed to respond to the market requirements are so different in the two cases. Airlines will offer an integrated service linking a few hubs to an extended network of secondary routes in order to get every client to his or her destination. Where needed, code sharing through strategic alliances with other airlines will do the trick of providing a comprehensive one-stop-only service. This is not at all the case when it comes to neutron facilities. All of them are extremely keen on being autonomous in their development and decision making processes. The client has to deal with all of them individually. For some scientific problems this will mean writing a large number of individual proposals sometimes for instrumentation of similar performance at different facilities. Code sharing of instruments is practiced only in very exceptional cases.

If we take a purely European perspective then undeniably progress has been achieved in the collaboration of neutron providers over the last decade. The Integrated Infrastructure Initiative NMI3 has played a vital role in this development. We are, however, far from real integration.

This becomes extremely obvious when monitoring the process of launching the next European flagship facility ESS. The decision on the ESS is prepared with limited attention given to how the new facility will fit into the existing ecosystem of neutron providers and neutron users apart from the fact that it will have to produce unprecedented experimental capabilities. This is a little bit like an airline reflecting on a new hub of unprecedented size without taking into consideration the network of existing airports and the geographical distribution and aspirations of the clients. It has unfortunately to be anticipated that the effort of inducing cohesion into the build-up of future European neutron infrastructure via the EU sponsored and ENSA coordinated Preparatory Phase Proposal will bear little fruit due to the lack of real political weight.

It is often argued that integration is a problem because it puts a break onto competition and thus delays progress. From a European perspective and in a global scientific environment this argument is rather weak. There is sufficient competition arising from the rest of the world due to top-of-the-range facilities that are coming on line in the United States and in Asia. In any case integration does not preclude internal competition if the resources committed are tensioned against performance. When two airlines merge they have all interest that both of their hubs keep the highest standards of service. If not one of them may disappear.

In a well-integrated European neutron infrastructure facilities should really play to their individual strength. When the ESS will become operational we will have at least four strong and complementary neutron hubs: The long pulse spallation source ESS, a powerful short pulse source at ISIS, and the two strongest reactor based sources at the ILL and FRM-II. The medium and smaller size sources will provide the important spokes necessary to stabilize the wheel of European neutron science.

But how will this ensemble really become an integrated neutron provider? At the moment not even the integration of the two truly European sources ESS and ILL has been mentally tackled. In the US the recently commissioned SNS and the high-flux reactor HFIR now present a common face to the outside world. Complementary instrument suites are offered to the user via a shared proposal and selection process. Ideas going in the same direction are developed between national neutron and synchrotron sources like BESSY and HMI. Do we really want to oblige future neutron users to write separate proposals for the ILL and the ESS? Do we want to maintain two separate scientific councils advising these two facilities without one knowing about the intentions of the other? Do we want to develop methods and techniques in splendid isolation both at the ESS and ILL? Do we really want European governments to choose between ESS and ILL in those cases where there community is too small to justify participation in both, thus limiting the instrument portfolio accessible to the users from these countries?

I guess the answer has to be no. Proceeding in this way would simply not constitute the most efficient way of transforming a given amount of public resources into scientific output. This becomes the more important as facilities have to provide more than neutrons.

Support laboratories for the different communities will place extra tension on the budgets. Wouldn't it be desirable in this context that we aim in the future towards a real European Neutron Network nucleated around a European Neutron Science Facility constituted in a first time by the two European neutron hubs ESS and ILL. Getting this integration of European neutron infrastructure off the ground will take political will and courageous decisions. If succes-

ful it may be a model for European infrastructure networking in the same way the ILL was an example for cross-national scientific collaboration. Others like the synchrotron community may follow suite. Many organizational forms are imaginable. ESS and ILL could become either fully integrated by possessing a common legal framework or more or less loosely bound, possessing common stakeholders and common decision making bodies, but staying otherwise autonomous. The later solution would make it particularly easy for other neutron providers (ISIS, FRM-II, HMI, LLB, PSI) but equally delocalized support laboratories to join the club. The renewal of the ILL intergovernmental agreement in 2013 may be the occasion for choosing the right track.

Independent of the organizational details the European Neutron Science Facility should provide a one-stop-shop for the user community. Cohesion of development and internal tensioning of resources have to be well balanced to preserve the highest possible standards of quality in an international competitive environment. Resources may be shifted gradually from one hub to the other following trends in scientific demand and performance. This explicitly includes the possibility that the ILL may be phased out beyond the horizon of 2030, e.g. at the profit of a European short pulse source (why not a 1 MW upgrade of ISIS).

We naturally can continue to work in the ways of the past pursuing our own individual routes. I am afraid that in this case we may miss an important opportunity. Spreading our resources too thinly and duplicating our services to the users may be good for competition. However, it equally bears the risk of remaining sub-optimum.



# Quantum oscillations of the total spin in a heterometallic antiferromagnetic ring

T. Guidi

HMI, Berlin, Germany

S. Carretta, P. Santini and G. Amoretti

University of Parma, Italy

R. Caciuffo

EC, JRC-ITU, Karlsruhe, Germany

A. Hiess, ILL

J.R.D. Copley and Y. Qiu

NIST Center for Neutron Research, USA

G. Timco and R.E.P. Winpenny

University of Manchester, UK

## ABSTRACT

The identification of systems displaying quantum coherence at the mesoscopic scale is of great interest, both from a fundamental scientific perspective, and in the context of potential technological applications in the field of quantum computation. Antiferromagnetic molecular rings are very interesting in this respect. Using inelastic neutron scattering (INS), with applied magnetic fields  $B$  up to 15 T, we have studied the spin dynamics of an important member of this class of materials,  $\text{Cr}_7\text{Ni}$ . We demonstrate that several avoided crossings (ACs), involving states with different total-spin quantum numbers, occur with increasing  $B$ . This corresponds physically to quantum oscillations of the total spin of the ring.

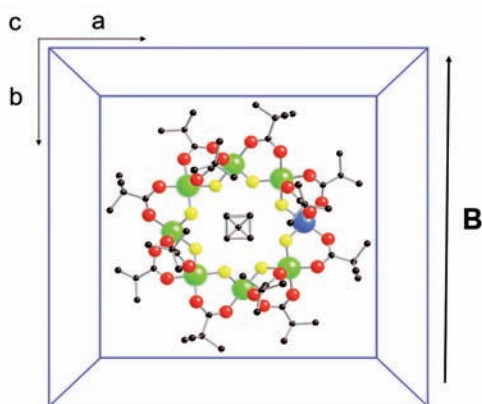
Antiferromagnetic (AF) molecular rings are cyclic clusters with dominant nearest neighbour AF coupling. When organised in a crystal lattice, they provide an ensemble of identical, almost non-interacting magnetic units [1] and represent very promising systems for the observation of quantum coherent phenomena. Among the wide class of AF rings synthesised so far, the  $\text{Cr}_7\text{Ni}$  heterometallic ring has been identified as a model system for the implementation of qubits [2]. This cyclic cluster has a  $S = 1/2$  doublet ground state, resulting from the dominant AF exchange interaction between seven Cr(III) ions ( $s = 3/2$ ) and one Ni(II) ion ( $s = 1$ ) (figure 1).

A doublet ground state, well separated from the first excited level, is one of the prerequisites for a system to be suitable for encoding a qubit. Another crucial condition is the persistence of quantum coherence during the time needed for the elementary computational operations to be performed. It is thus important to know in great detail the quantum spin dynamics of these systems to better understand to what extent their properties match the desired ones.

The application of an external magnetic field  $B$  enables the energies and the composition of the eigenstates from the ring's Hamiltonian to be tuned. In particular, in  $\text{Cr}_7\text{Ni}$  several “avoided crossings” (AC) between different spin states are induced by a field with appropriate value and direction. When AC conditions are met, two different spin states are superimposed, and the total spin of each ring oscillates in time between  $S$  and  $S+1$  [3].

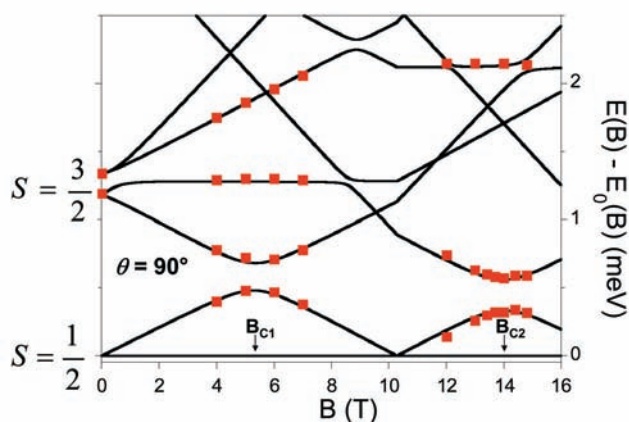
Using the Disk Chopper Spectrometer at NIST, we have observed this phenomenon around an AC that involves the spin ground state [3].

The three-axis spectrometer IN14 was then used to study the spin dynamics at AC conditions involving excited spin states, and to investigate the effects of the AC on the composition of the spin wavefunctions. For this experiment, we used a 0.4 g single crystal sealed in a preservative HF/MeCN(1:2) atmosphere within an aluminum sample holder. A 15 Tesla vertical-field cryomagnet was used to apply a magnetic field parallel to the ring plane (figure 1). With fixed final neutron wave vector  $k_F = 1.15 \text{ \AA}^{-1}$ , and a base temperature of 1.5 K, we collected inelastic constant  $Q$  scans, at different magnetic fields around the



**Figure 1.** Schematic view of the  $\text{Cr}_7\text{Ni}$  molecular structure in the unit cell (view direction parallel to the crystallographic  $c$  axis). Cr: green spheres, F: yellow, O: red, C: black; Ni, blue, disordered over the 8 sites of the ring. H atoms are omitted for clarity. The experiment on IN14 was performed with the magnetic field lying in the plane of the ring.





**Figure 2.** Calculated field-dependence of the low-lying energy levels of  $\text{Cr}_7\text{Ni}$ , relative to the ground-state energy, for an angle  $\theta=90^\circ$  between the applied magnetic field and the anisotropy axis  $c$ . Points indicate the positions of the observed INS peaks. AC conditions occur in correspondence of magnetic field amplitudes  $B_{C1}$  and  $B_{C2}$  (arrows).

ACs. The modulus of  $Q$  was chosen close to the value corresponding to the maximum of the magnetic intensity as a function of  $Q$  [4].

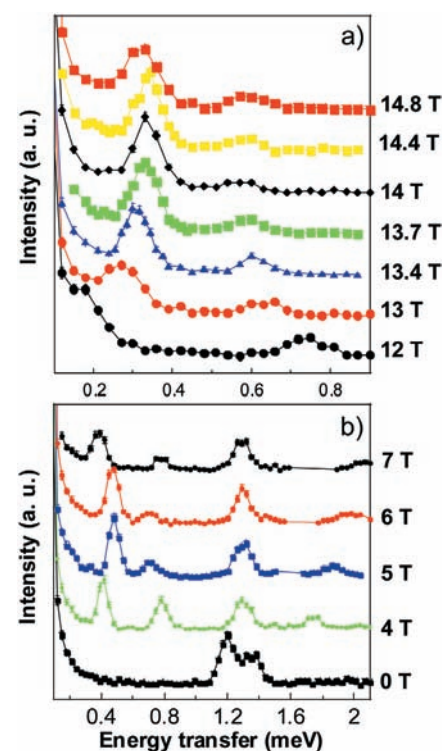
In figure 2 the energies of the observed excitations are compared against the calculated energy level scheme as a function of the magnetic field. The occurrence of ACs between the first and second excited spin states at  $B_{C1}=5.3\text{T}$  and  $B_{C2}=14\text{T}$  is evidenced by the field dependence of the observed excitations and by the very good agreement with the theoretical calculations.

The spectrum at 0 T in figure 3b shows the transition from the  $S = 1/2$  ground state to the  $S = 3/2$  first excited state, split by anisotropic spin-spin-interactions and uniaxial local crystal fields. Increasing the field, we were able to follow the Zeeman shift of the low temperature excitations in the field interval corresponding to the AC fields  $B_{C1}$  (figure 3b) and  $B_{C2}$  (figure 3a).

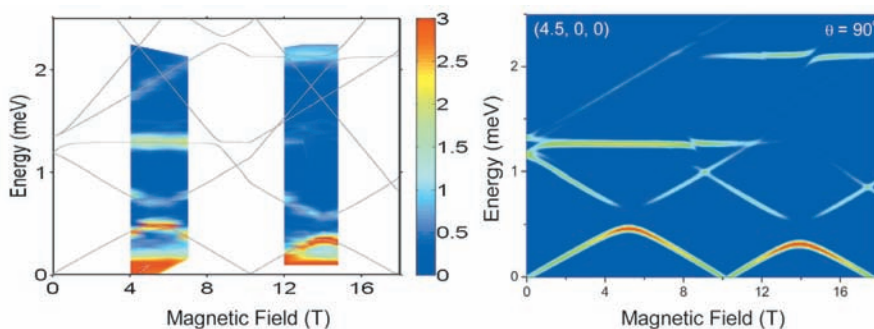
The mixing of different spin states at the AC condition also affects the intensities of the observed excitations. Figure 4 shows a plot of the INS cross section as a function of magnetic field and energy transfer. For magnetic fields approaching  $B_{C1}$  and  $B_{C2}$ , a redistribution of the INS intensity is observed, providing additional insight into the readjustment of the spin wavefunctions in the vicinity of the AC condition.

In conclusion, high field INS measurements on a  $\text{Cr}_7\text{Ni}$  single crystal have demonstrated the occurrence of avoided crossings involving states with different total-spin quantum numbers. The INS cross section shows an enhancement of the effect of the superposition of different states at the AC condition,

**Figure 3.** Constant  $Q$  scans for  $Q=(4.5, 0, 0)$  r.l.u. (reciprocal lattice units), varying the incident energy (fixed  $k_F=1.15 \text{ \AA}^{-1}$ ) at different magnetic fields near the AC conditions ( $T=1.5 \text{ K}$ ). The data are vertically offset for clarity. The modulus of  $Q$  was chosen close to the value where the magnetic intensity has its maximum [4].



**Figure 4.** Intensity plot showing energy and field dependence of the measured (left) and calculated (right) INS cross sections for  $\theta=90^\circ$  and  $Q=(4.5, 0, 0)$  r.l.u.;  $T=1.5 \text{ K}$ .



where quantum oscillations of the total spin of the molecule take place. The very good agreement for the positions and intensities of the observed excitations with calculations gives us confidence in the validity of the model spin Hamiltonian and permits further speculations and predictions as to the feasibility of quantum information processing using this class of molecules.

## REFERENCES

1. F.K. Larsen et al., *Angew. Chem. Int. Ed* 42, 101 (2003). R.H. Laye et al., *Chem. Commun.* 1125 (2005). M. Affronte, et al., *Chem. Commun.*, 1789 (2007) and references therein.
2. F. Meier, J. Levy and D. Loss, *Phys. Rev. Lett.* 90 (2003) 47901; F. Troiani et al., *Phys. Rev. Lett.* 94 (2005) 207208.
3. S. Carretta et al., *Phys. Rev. Lett.* 98 (2007) 167401 and references therein.
4. R. Caciuffo et al., *Phys. Rev. B* 71 (2005) 174407.



# Neutron tomography in modern archaeology

**N. Kardjilov, A. Hilger and I. Manke**

Hahn-Meitner-Institut Berlin  
Glienicker Str. 100, D-14109 Berlin, Germany

**V. Benfante, F. Lo Celso and R. Triolo**

Università degli Studi di Palermo  
V.le delle Scienze - Pa.d. 17, 90128 Palermo, Italy

**I. Ruffo**

I.T.I. Vittorio Emanuele III  
V. Duca della Verdura 48, 90134 Palermo, Italy

**S. Tusa**

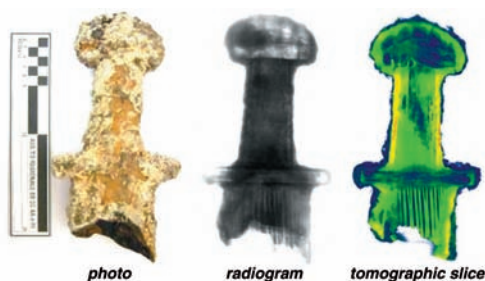
Soprintendenza del Mare, V. Lungarini 9  
90133 Palermo, Italy

## ABSTRACT

The search for non invasive and non destructive techniques is fundamental when dealing with samples of great historical, cultural and artistic value as well as with samples strongly degraded. Among different techniques, Neutron Tomography (NT) allows a close analysis of samples of Archaeological interest without damaging them. In what follows, a few cases in which the Neutron Tomography instrument of the BENSC at HMI (Berlin) has been successfully applied will be shown.

## INTRODUCTION

The use of Neutron Tomography for archaeometric investigations is quite recent. The first neutron tomography results for non-destructive investigation on archaeological samples were reported in 1996 [1]. In the following years a growing number of tomography measurements with neutrons have been performed on such kind of samples [2,3]. One of the key reasons of this success is the fast development in digital image recording and processing, which enables the computation of tomographic reconstructions from high-resolution images at a reasonable timescale. The development of new detectors with better signal-to-noise characteristics and faster read-out electronics has allowed the overcoming of some of the spatial and time resolution limitations of conventional neutron radiography and tomography. On the other hand, the property of neutron to easily transmit through large, dense samples is of great importance in modern archaeology. In fact, the three dimensional visualisation of the inner structure of samples of archaeological interest helps to understand the technological process of manufacturing or provides information about the source of materials used in ancient masterpieces, especially noble metals [4]. Therefore, it is not surprising the growing interest of the scientific community towards the use of NT for archaeometric investigations. The neutron probe shows its advantages, as well as complementarities, with respect to classical X-rays investigation techniques, especially when materials containing hydrogen are investigated. Indeed the high sensibility of neutrons for some light elements (for example H, Li, B) solves most of the interpretation problems arising from samples characterized by the presence of polymeric or aqueous components. For this reason another application of NT in modern archaeology is the non-destructive inspection of the quality of specimens for conservation purposes [5]. In such a case, due to the high sensitivity of neutrons to hydrogenous materials, neutron tomography allows visualization of the distribution of impregnating solutions, for example, in treated woods and/or in partially corroded metal matrices.



**Figure 1.** Investigation of the handle of a late Roman sword (left) by NT technique. A two-dimensional transmission image by neutrons is shown in the middle. A single slice from the 3D-tomographic volume is shown on the right. The color scale corresponds to the presented attenuation coefficients for neutrons from blue (hollow space) to red (iron). The green part represents the distribution of dissolved iron (Iron oxide).

## EXPERIMENTAL

The NT experiments, whose results will be described in what follows, have been performed at the Neutron Tomography instrument CONRAD of the Berlin Neutron Scattering Center (BENSC) at the Hahn-Meitner Institute (HMI,

Berlin). The cold neutron beam with a flux of approximately  $10^7$  neutrons/cm<sup>2</sup>s allows for transmission of solid samples with calcareous concretion shell of up to 8 cm. The beam size of 10 cm x 10 cm is sufficient for simultaneous investigation of a large number of small samples, or for single samples of reasonable size. A scanning system helps to investigate larger samples of up to 20 cm x 30 cm (width x height). The achieved spatial resolution varies between 50  $\mu$ m and 250  $\mu$ m depending on the detector settings. For the 3D tomographic reconstruction of the sample volume a number of 2D projections taken with the sample rotating over 180° or 360° is used as input in sophisticated mathematical (filtered back projection) algorithm. The number of projections depends on the sample size and is in the order of 300 to 600 single images taken in a few (3-4) hours of measuring time. The data can be visualized by means of special rendering software [6] as shown in the following figures. More details about the instrument can be found elsewhere [7].

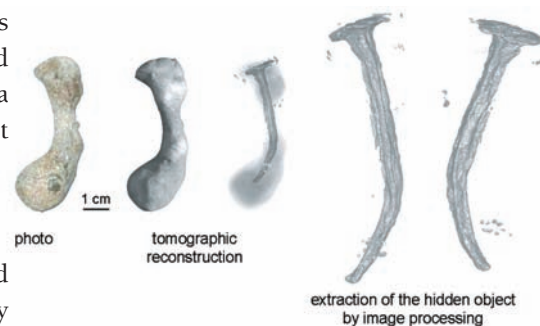
#### NT OF HIDDEN OBJECT AND OF RECOVERED UNDERWATER OBJECTS

The Neutron Tomography tool might be of extreme importance for obtaining the digital 3D reconstruction of recovered underwater items before starting the restoration work. First of all, the restoration and conservation work might be helped by the high resolution of the digital images, avoiding therefore wrong removal procedures of the calcareous concretion matrix of objects. In addition other precious information might be obtained for evaluating the degree of embedding of the concretion matrix inside and outside the object and the damages caused to the metallic parts, deciding whether or not the restoration work can take place (the metallic parts might collapse after years under water). Fig. 1 shows the tomographic reconstruction of a portion of a late Roman sword from ship wrecks in an area not far from Sicily southern coast characterized by a dangerous cliff (Scoglio della Bottazza).

Another example of application of NT in this context, is shown in Fig. 2, where the tomographic volume of the hidden object (a nail) inside a calcareous concretion shell has been extracted. Still there are many other objects that need to be recovered from the sea and the NT technique might help in building a database for identifying the correct historical frame period and also the correct conservation approach.

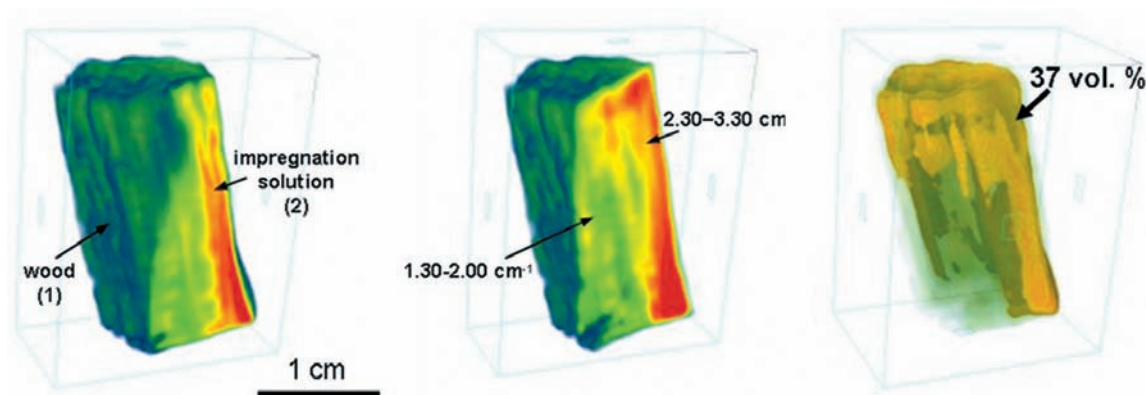
#### NT OF WATERLOGGED WOODS

NT may be of great help in the optimisation of techniques for preservation and conservation of waterlogged woods. Due to the high contrast provided by hydrogenous impregnating solution, the dynamics of its penetration inside the wood matrix can be observed three-dimensionally by means of NT. By varying the composition of the impregnating solutions or by applying different injection pressures the most appropriate conservation procedure can be adapted to the corresponding wood. Therefore, NT can provide extra quantitative information which can be used to estimate the efficiency of the treatment for waterlogged woods. An example of this is shown in Fig. 3 where a piece of wood has been preserved by an impregnating solution containing high molecular weight PEG. The NT reconstruction shows high contrast



**Figure 2.** NT investigation of an object inside a calcareous concretion shell. The photo of the sample is shown on the left. The tomographic volume of the extracted nail is shown in the three images following the tomographic reconstruction of the object.





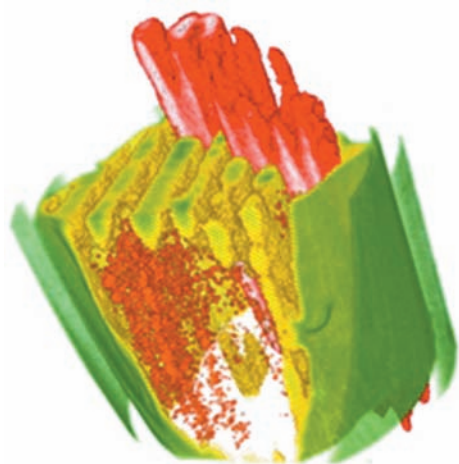
**Figure 3** Tomographic slices of impregnated wood. The attenuation coefficients for the solution (red) and the wood (green) are shown in the left and middle images and the calculated volume fraction of the solution and its distribution in the wood matrix are shown in the right image [2].

In this experiment a detector setup with higher resolution was used. The different portions have been highlighted and locally selectively eliminated, by means of a special rendering software [6], in order to better show the distribution of the different parts and of the impregnating solution inside the wood.

In order to resolve the wood structure with higher resolution and to be able to detect any changes in the wood matrix due to the impregnation process, X-ray micro Tomography measurements can be performed simultaneously.

**NT OF MARBLES AND STONES**

Another application of NT is in the investigation of stones and marbles. Among the natural composites, there is a wide variety of stones used in buildings, monuments, statues and other objects of archaeological or cultural heritage interest. Sandstone, Limestone, Granite and Marbles are the most common stones used for these purposes. Clearly it is of archeological interest to link certain



**Figure 4** Tomographic reconstruction of impregnated wood. The colours for the solution (red) and the wood (yellow-green) are related to the corresponding attenuation coefficients.

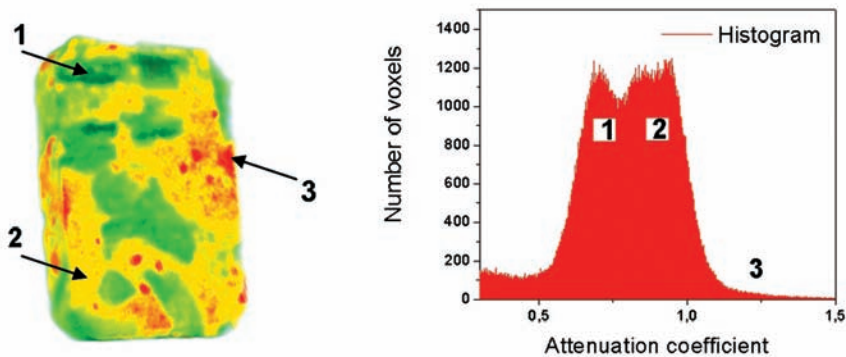
**Table I**

Phase, No.	1	2	3
Attenuation coeff., cm <sup>-1</sup>	0.50-0.80	0.80-1.10	1.10-1.50
Volume fraction, %	40	58	2

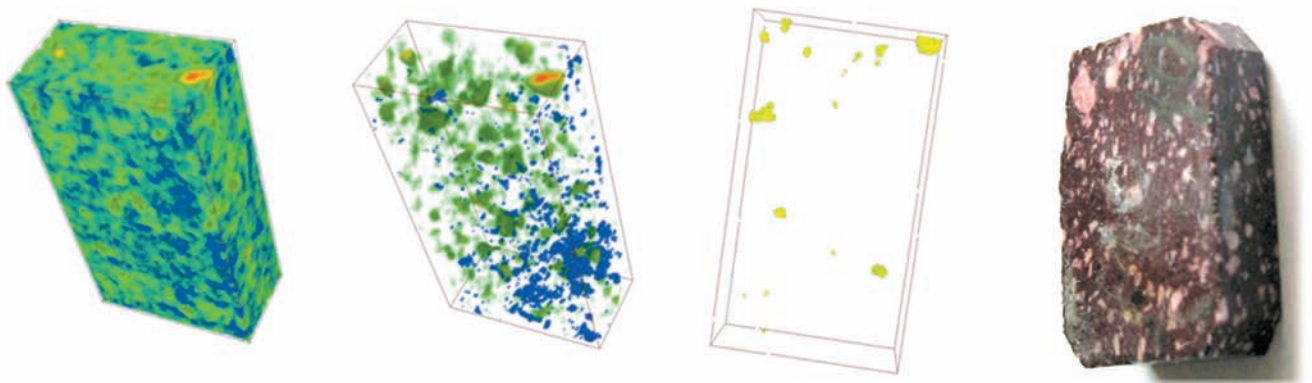
types of marbles to the areas and formations they have been taken from. An example of the information which can be obtained by means of NT is shown in the following Fig. 5 [5]. The sample is a polychromic marble from Villa Adriana (Tivoli, Italy). The tomographic image is shown on the left. The histogram plot is presented on the right side. The stone shows the presence of three phases described in the Table I. The different phases are indicated in the tomographic image as well as in the histogram plot by numbers.

Figure 6 shows a similar three component polychromic stone from Villa Adriana, whose picture is on the right side of the figure.

The sequence of 3D reconstructions shows on the left the three components, identified by the green, blue and yellow-orange colours. As it can be noticed, the amount of one of the components is extremely low, and yet still identifiable by NT. Also in this case, in order to resolve the stone structure with higher resolution, X-ray micro Tomography (XmT) measurements can be performed simultaneously. A dramatic increase in resolution can be achieved with this technique. However, the size of the samples which can be investigated is necessarily much smaller.



**Figure 5** Morphological study of a polychromic stone.



**Figure 6.** A three component polychromic stone from Villa Adriana (Tivoli)

#### ACKNOWLEDGEMENTS

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#### REFERENCES

1. B. Schillinger, R. Gebhard, B. Haas, W. Ludwig, C. Rausch, U. Wagner, 3D Computer tomography in Material Testing and Archaeology, presented at the 5th World Conference on Neutron Radiography Berlin, Germany, June 17-20, 1996.
2. J. Rant, A. Rant, Z. Mili, G. Rihar, Applications of Neutron radiography in Archaeology, presented at the 15th World Conference on Non-Destructive Testing 15-21 October 2000 in Rome.
3. E. Lehmann, P. Vontobel, L. Tobler, L. Berger, E. Deschler-Erb, A. Voûte, Non-destructive Studies of Archaeological Objects Using Neutron Techniques, NUM Progress Report 2002, <http://num.web.psi.ch/reports/2002/pdf/e-19.pdf>.
4. N. Kardjilov, F. Fiori, G. Giunta, A. Hilger, F. Rusticheli, M. Strobl, J. Banhart, R. Triolo, Neutron tomography for archaeological investigations, *Journal of Neutron Research* 14 (2006) 29-36
5. N. Kardjilov, F. Lo Celso, D. I. Donato, A. Hilger, R. Triolo, Applied neutron tomography in modern archaeology, *Il Nuovo Cimento* 30 (2007) 79-83
6. More information: [www.volumegraphics.com/](http://www.volumegraphics.com/)
7. See: [www.hmi.de/bensc/instrumentation/pdf\\_files/BENSC\\_V7.pdf](http://www.hmi.de/bensc/instrumentation/pdf_files/BENSC_V7.pdf).



# Inelastic neutron scattering measurement of hydrogen single-molecule dynamics in clathrate-hydrates

L. Ulivi, M. Celli, A. Giannasi, M. Zoppi  
Istituto dei Sistemi Complessi, CNR, Via Madonna  
del Piano 10, 50019 Sesto Fiorentino, Italy

A.J. Ramirez-Cuesta  
ISIS at RAL, Chilton, Didcot, UK

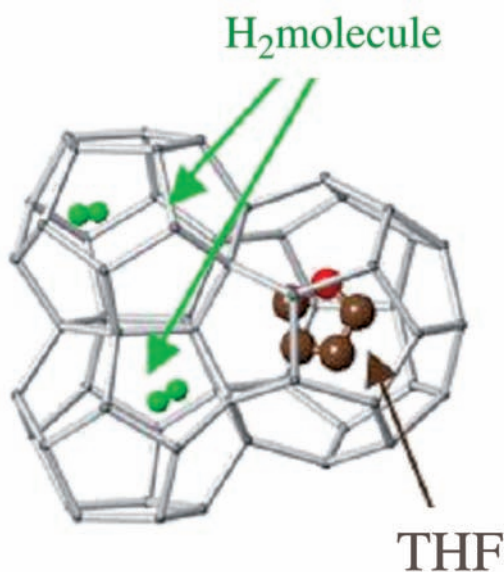
## ABSTRACT

We discuss a high-resolution inelastic neutron scattering experiment on hydrogen-tetrahydrofuran clathrate hydrates, where the  $H_2$  molecules are enclosed in cavities formed by the solid water lattice. The spectrum due to the  $H_2$  molecule excitations is very intense with respect to that of the deuterated lattice excitations, and shows spectral bands that are assigned unambiguously to rotational transitions, center-of-mass translational transitions of either para- or ortho- $H_2$ , and to combinations of these. We demonstrate that the  $H_2$  molecule rotates almost freely, and performs a translational motion (rattling) in the cage, which is a paradigmatic example of the motion of a quantum particle in a non-harmonic three-dimensional potential well. A simple isotropic model for the rattling motion enable us to calculate the energy levels and the neutron energy loss spectrum for both p- $H_2$  and o- $H_2$  transitions, which is compared with our experimental results. The resulting agreement is good, considering the approximations in the calculation, and confirms the assignment of the observed bands.

Clathrate-hydrates (also known as gas hydrates) are an important kind of water inclusion compounds.<sup>1</sup> The name stems from the Greek κλειθρον (kleithron, meaning bar or fence) and from the Latin “clatratus” (closed with bars).

In these solids, the largest part is water, and the other components are constituted by molecules that do not form a chemical bond with water. These may be molecules of a natural gas (as methane, ethane, propane), a noble gas, or a hydrocarbon. The gas molecules (guests) are trapped in cavities formed by the hydrogen-bonded water lattice, which have different geometrical form. Guest molecules have the function of stabilizing the lattice in a structure quite different from that of any form of ice, and, in turn, the clathrate would not be stable without guest molecules. The fact that the melting temperature (at a moderate pressure) for these solids is generally higher than that for hexagonal ice Ih is an indication that these crystals are more stable than ice. In other words, water, in the presence of a foreign gas crystallizes preferentially in the form of clathrate than into that of normal ice. These compounds are overwhelmingly present in nature. It is known that methane-hydrates are present in ocean depths or in onshore deposits, and these are considered an important energy resource.<sup>1</sup> Solid methane-hydrate also forms in gas pipelines, where is a source of problems and danger, since it can induce plugging of the pipeline.

Depending on guest's type and dimension, the hydrate crystal structure can attain one among essentially three different structures, two of which are cubic and one hexagonal, which are named cubic structure one and two (sI and sII) and structure H (sH), respectively. The crystal structure is well known in all three cases. The crystal can be pictured as being formed by joining together the cavities where the guest molecules are hosted. These have the form of polyhedra, whose faces are (almost regular) pentagons, hexagons or squares. A notation commonly used for designating a cavity shape is a sequence of integer



**Figure 1.** Schematic drawing of the small and large cages of a THF- $H_2$  clathrate. One oxygen atom is located on each vertex of the polyhedra, which represent the water lattice, and is tetrahedrally coordinated. Each side represents an hydrogen bond.

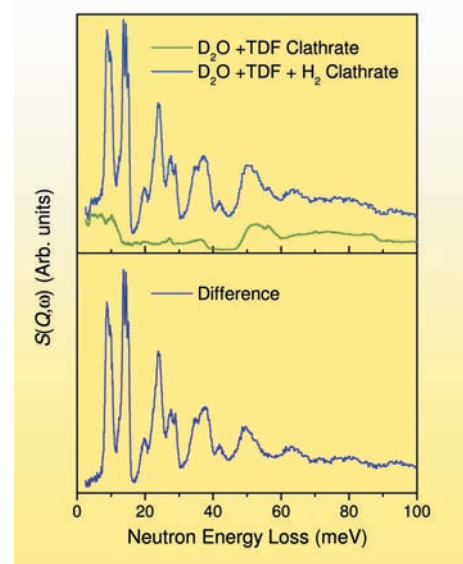
numbers each elevated at an integer power, as, for example,  $5^{12}6^2$ , indicating polyhedra with 12 pentagonal faces and two hexagonal faces. The  $5^{12}$  cage, that is a regular dodecahedron, is present in all clathrate structures. Cubic sI clathrates are formed by  $5^{12}$  and  $5^{12}6^2$  cages, while three types of cages concur to the formation of hexagonal sH clathrates, namely  $5^{12}$ ,  $5^{12}6^8$ ,  $4^35^66^3$ . We will be dealing with clathrates having the sII structure, which we describe in somewhat greater detail. Cubic sII clathrate has a unit cell with 132 water molecules, that form 16 dodecahedral cages ( $5^{12}$ ) and 8 larger cages shaped as a polyhedron (hexakaidecahedron) with 12 pentagonal and 4 hexagonal faces ( $5^{12}6^4$ ). The (average) radii of the cages hardly depend on the guest molecules, and are 3.95 Å and 4.33 Å respectively. The space group for this structure has been determined and is Fd3m. It is known that gases as Ar, Kr, O<sub>2</sub>, N<sub>2</sub>, propane and liquids as tetrahydrofuran (C<sub>4</sub>H<sub>8</sub>O) form this type of hydrate.

Hydrogen molecule has long been thought to be too small to stabilize water into one of the solid clathrate structures, until a H<sub>2</sub> clathrate was discovered, which is formed at a pressure of about 200 MPa.<sup>2</sup> This clathrate was subsequently studied experimentally<sup>3,4</sup> and theoretically,<sup>5</sup> for the strong interest it raised in view of hydrogen storage applications. As a matter of fact, even though it is estimated that the H<sub>2</sub> content for this compound is only of the order of 4-5 % in weight, the fact that the only other component is water makes it particularly appealing on environmental grounds. The search of other similar compounds with lower synthesis pressure led to the discovery of a water-hydrogen-tetrahydrofuran (THF) clathrate, which is formed at around 10-20 MPa.<sup>6</sup> This clathrate has the same sII crystal structure, with 16 small and 8 large cages per unit cell, but here the large  $5^{12}6^4$  cages are occupied by THF molecules (see Fig. 1). The H<sub>2</sub> storage capability is therefore somewhat reduced. In contrast to what initially believed<sup>4,6</sup> the small cage hosts only one H<sub>2</sub> molecule.<sup>7</sup>

Clathrates are also intriguing compounds for fundamental physics. Although they are regular ordered crystalline solids, the dynamics of the guest molecule is different from the other normal modes of the water lattice, having the character of nearly localized vibration into the confines of the nearly spherical cage, which is known as rattling. The coupling of this motion with the phonons of the crystal is considered to be the main cause of the anomalous glass-like thermal conductivity discovered in these systems.<sup>8</sup>

In this report we discuss the results of inelastic neutron scattering (INS) measurements on hydrogen-tetrahydrofuran clathrate, performed with the aim of measuring the dynamics of the H<sub>2</sub> molecule inside the cage.<sup>9,10</sup> The experiment was performed on the high resolution inverted-geometry neutron spectrometer TOSCA at the pulsed neutron facility ISIS (U.K.).<sup>11,12</sup> The neutrons scattered at two fixed angles (42.6° and 137.7°), and at a fixed final energy of 3.3 meV are recorded, providing a neutron energy loss spectrum between  $E=3.5$  meV to about  $E=1000$  meV. In the range of our interest (below about 150 meV) this instrument has an energy resolution probably unattained by any other similar neutron instrument in the world, namely  $\Delta E/E < 2.5$  %.

Inelastic neutron scattering presents a very high sensitivity when applied to the study of materials that contain hydrogen due to the particularly large incoherent scattering cross-section of the proton, which is much greater than

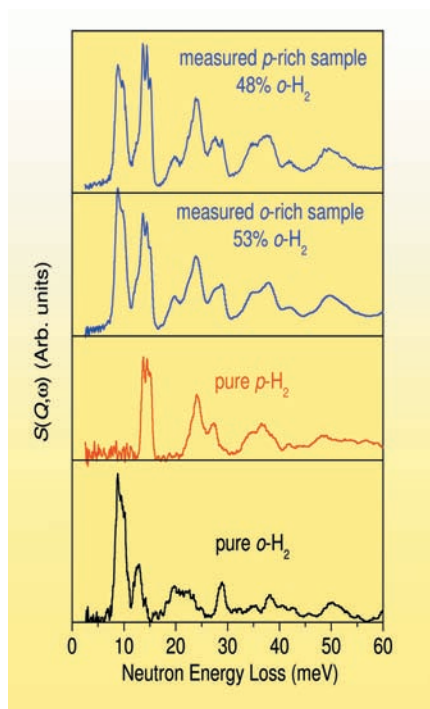


**Figure 2.** Upper panel: neutron energy loss spectra of a TDF-D<sub>2</sub>O clathrate recorded on TOSCA (green line) compared with that of a H<sub>2</sub>-TDF-D<sub>2</sub>O clathrate. Lower panel: Spectrum obtained by difference after normalization for the different sample masses.





**Figure 3.** Two upper panels, blue: neutron energy loss spectrum measured at 20 K on two different H<sub>2</sub>-TDF-D<sub>2</sub>O samples, with 48 % and 53 % *o*-H<sub>2</sub> concentration, respectively, after subtraction of the TDF-D<sub>2</sub>O background spectrum. Two lower panels: spectra of H<sub>2</sub>-TDF-D<sub>2</sub>O clathrates containing *p*-H<sub>2</sub> (red) or *o*-H<sub>2</sub> (black) only, derived as explained in the text.



that of any other nucleus. This allows a relatively simple access to the self dynamics of trapped molecular hydrogen (H<sub>2</sub>). For this reason, samples for the present experiment were produced using D<sub>2</sub>O and completely deuterated tetrahydrofuran (TDF). These two liquids were mixed in stoichiometric proportion (17:1 mol), enclosed in a beryllium-copper autoclave where hydrogen gas at about 800 bar was added. The liquid mixture was then slowly frozen at a temperature between 0 °C and +2 °C, applying a continuous stirring. Alternatively, samples were produced by preparing first a TDF-D<sub>2</sub>O solid clathrate, grinding it to a fine powder, and then keeping it, for a time of the order of 24 hours or more, into the autoclave with H<sub>2</sub> at a pressure around 1000 bar and temperature of a few degrees below 0 °C. Once the clathrate is formed, it is quenched, by immersing the autoclave into liquid nitrogen, the pressure is released, and the sample is recovered. All subsequent sample manipulations are done at about 77 K and under dry nitrogen atmosphere, to avoid contamination with atmospheric H<sub>2</sub>O vapor. We have noted that the second preparation procedure produces samples with a quite higher H<sub>2</sub> content, which we have estimated, from gas release thermodynamic measurements, to be consistent with the hypothesis of single H<sub>2</sub> occupancy of the totality of the small cages. In this report we discuss the results obtained from two gas-charged samples, which had a different para-H<sub>2</sub> (*p*-H<sub>2</sub>) and ortho-H<sub>2</sub> (*o*-H<sub>2</sub>) concentration, prepared starting with either normal H<sub>2</sub> or almost pure *p*-H<sub>2</sub>. Additionally, we prepared one simple TDF-D<sub>2</sub>O clathrate as a reference sample. Due to the procedure of sample preparation (close to room temperature), quenching at 77 K and subsequent preservation at the same temperature, the *o*-H<sub>2</sub> concentration with respect to *p*-H<sub>2</sub> in our two hydrogenated samples was not much different, resulting 48% (*p*-rich sample) and 53% (*o*-rich sample). This has been derived by comparing the intensity of the S<sub>0</sub>(0) and S<sub>0</sub>(1) rotational lines in the Raman light scattering spectrum measured in our laboratory, before and after the neutron experiment. Even if the difference is small, the comparison of the neutron spectra of the *p*-rich and *o*-rich samples has been the key issue for the interpretation of the spectral features, allowing the separation of the measured spectrum into the sum of the excitations of the *p*-H<sub>2</sub> and of the *o*-H<sub>2</sub> molecules, as described in the following. Neutron measurements were performed at a temperature  $T=20$  K.

We present in Fig. 2 (upper panel) a comparison between the neutron spectra of the reference TDF-D<sub>2</sub>O clathrate (green line) and the *p*-rich sample (blue line). It is evident how much the scattered neutron intensity increases when hydrogen is present into the clathrate. The lower panel of Fig. 2 shows the difference of the two spectra. The discussion that follows refers to the spectra where the “background”, that is the spectrum of the TDF-D<sub>2</sub>O clathrate, has been subtracted, after a suitable normalization that takes into account the mass of the sample exposed to neutrons and the total neutron flux of each set of measurements. Essentially, the bands represent the excitations of the H<sub>2</sub> molecule inside the small cage of the clathrate.

In Fig. 3 we show the comparison of the spectra measured for the *p*-rich and *o*-rich spectra. We note, by observing the two upper panels of Fig. 3, that one important difference is related to the intensity ratio between the two bands at ≈10 meV and ≈14 meV (in this order), which is *higher* in the *o*-rich sample.

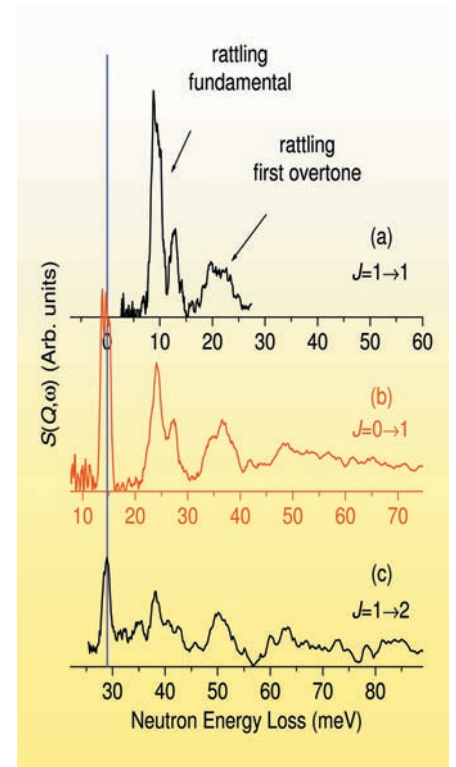


This already indicates that the band at  $\approx 14$  meV is related to the presence of  $p$ -H<sub>2</sub> while the one at  $\approx 10$  meV is due to  $o$ -H<sub>2</sub>. With an eye to Fig. 3, it is then easy to understand how the spectrum has been decomposed into the sum of the  $p$ -H<sub>2</sub> and  $o$ -H<sub>2</sub> spectra. As a matter of fact, since the  $o$ -H<sub>2</sub> and  $p$ -H<sub>2</sub> concentrations into the clathrate are known, the two spectra of the pure species are simply derived by a linear combination of the signal measured for the  $p$ -rich and  $o$ -rich clathrates. These are shown in the two lower panels of Fig. 3. The good signal-to-noise ratio in the original measurements has the effect that also in their difference the excitation bands are determined with high accuracy. Two features are readily recognizable in spectra. These are the band at  $\approx 14$  meV in the  $p$ -H<sub>2</sub> clathrate spectrum, which correspond to the excitation from the rotational state  $J=0$  to  $J=1$  of a  $p$ -H<sub>2</sub> molecule, and the weaker band at  $\approx 28$  meV in the  $o$ -H<sub>2</sub> spectrum, corresponding to the  $J=1 \rightarrow 2$  rotational transition of an  $o$ -H<sub>2</sub> molecule. Similar sharp bands due to molecular rotational transition have been observed in solid hydrogen.<sup>13</sup> The presence of these rotational bands is a demonstration of the almost free rotation of the H<sub>2</sub> molecule in the cage, and the near coincidence of the average position of the bands with what we calculate for a free molecule indicates that the rotational states of H<sub>2</sub> are only weakly perturbed by the interaction with the water molecules of the cage. The other bands that are present in the spectra are to be assigned to excitations pertaining to the center-of-mass (CM) motion, or to combinations of these with molecular rotations, as it will be described in the following.

To render this analysis more quantitative, we discuss the approximations that allows us to identify the measured neutron loss energy spectra with the self part of the dynamical structure factor of the H<sub>2</sub> molecules in the clathrate. First, we need to consider the neutron scattering cross section for the  $p$ -H<sub>2</sub> and  $o$ -H<sub>2</sub> species, and its dependence on the rotational transitions.<sup>14</sup> The treatment of the neutron scattering from a light molecular species like H<sub>2</sub> usually relies on the approximations of considering the translational motion as independent of the internal (rotational and vibrational) degrees of freedom, and independent of the spin<sup>15</sup> This treatment allows one to write, for the double differential neutron scattering cross section, the relation

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{k_f}{k_i} \left[ S_d^{CM}(\mathbf{Q}, \omega) u(\mathbf{Q}) + S_{self}^{CM}(\mathbf{Q}, \omega) \otimes v(\mathbf{Q}, \omega) \right] \quad (1)$$

where  $k_i$  and  $k_f$  denote the initial and final neutron wavevectors,  $\omega=E/\hbar$ , and the symbol  $\otimes$  denotes a convolution product. The quantities  $S_d^{CM}(\mathbf{Q}, \omega)$  and  $S_{self}^{CM}(\mathbf{Q}, \omega)$  are the distinct and self part of the dynamic structure factor for the CM motion.<sup>14</sup> Equation (1) is the generalization to a molecular system of the usual separation into a self and distinct part of the dynamic structure factor for a mono-atomic system. In the case of H<sub>2</sub> one can make the additional approximation of neglecting the coherent part of the nuclear cross section with respect to the incoherent one. This leads to neglecting the first term in the square bracket of Eq.1, since the factor  $u(\mathbf{Q})$  is proportional to the coherent cross section only. The intensity factor  $v(\mathbf{Q}, \omega)$  depends on the intra-molecular modes, and is expressed by simple relations in the case of separation of



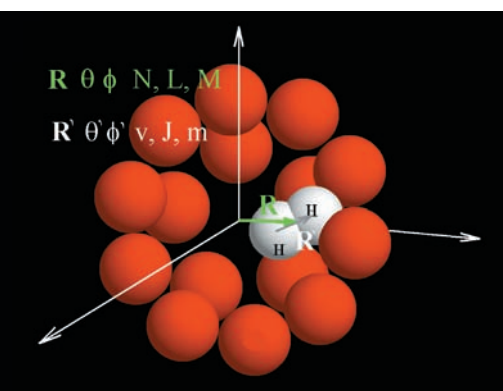
**Figure 4.** (a)  $o$ -H<sub>2</sub> spectrum, limited to the region below 29 meV; (b)  $p$ -H<sub>2</sub> spectrum, (red) shifted by  $\Delta E_{01} = 14.7$  meV, and (c)  $o$ -H<sub>2</sub> spectrum shifted by  $\Delta E_{12} = 29.0$  meV. The coincidence, in frequency and shape, of the rattling fundamental and first overtone in the three spectra is evident.



rotational and vibrational degrees of freedom. For a vibrating rotor, the  $\omega$ -dependence of  $v(\mathbf{Q},\omega)$  is in the form of a sum of Dirac  $\delta$ 's, one for each vibro-rotational state of the molecule. Since in our case the explored energy range does not cover  $H_2$  vibrational transitions, we will consider only rotational transitions, and we will write

$$\left(\frac{d^2\sigma}{d\Omega d\omega}\right)_s \equiv \frac{k_f}{k_i} \sum_{rot} S_{self}^{CM}(\mathbf{Q},\omega) \otimes \delta(\omega - \omega_{JJ'}) b^2(J,J') f(J,J',\mathbf{Q}) \quad (2)$$

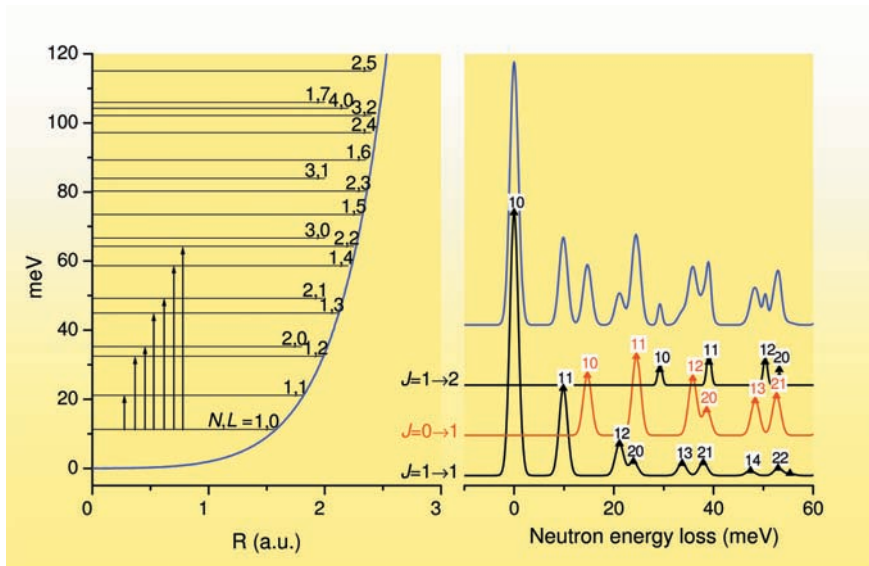
The Dirac  $\delta$ -functions are centered at the energies of the rotational transitions,  $\hbar\omega_{JJ'}$ , of the  $H_2$  molecule and the intensity factor  $f(J,J',\mathbf{Q})$  is a function of the momentum transfer  $\mathbf{Q}$  and depends on the rotational transition  $J \rightarrow J'$  of the molecule. The expected spectrum therefore consists of the CM excitations replicated and shifted by the energy of any possible rotational excitation of the molecule. Since INS is not subject to selection rules, all transitions to molecular rotation and vibration states are allowed. In addition, modeling the molecule as a rigid rotor, or a freely rotating harmonic oscillator, the intensity factors  $f(J,J',\mathbf{Q})$  can be easily calculated.<sup>15</sup> The expected spectrum is therefore the sum of several replicas of the CM dynamical structure factor  $S_{self}^{CM}(\mathbf{Q},\omega)$ . These replicas are as many as the (significant) rotational transitions of the molecule, they are shifted by the rotational transition energy of the molecule and their intensity is scaled by the known factor  $f(J,J',\mathbf{Q})$ . In other words, using a spectroscopic terminology, we can say that the spectrum contains all the rotational transitions of the molecule, and, in addition, the *combination bands* of each rotational transition with the CM excitations. On the other hand,  $S_{self}^{CM}(\mathbf{Q},\omega)$  itself should consist of a spectrum of lines, since it pertains to a localized motion of a quantum particle in a potential well. At 20 K, the experimental temperature, only the lowest rotational states (i.e.  $J=0$  and  $J=1$ ) are populated, and the rotational transitions to be considered are essentially three. For *o*- $H_2$ , the elastic  $J=1 \rightarrow 1$  transition should give a band centered at zero energy transfer (which is outside of the explored energy range) followed, at higher energy, by its combinations with the CM excitations. The same is expected to happen for the inelastic *o*- $H_2$   $J=1 \rightarrow 2$  transition (at 29.0 meV). For *p*- $H_2$ , the elastic  $J=0 \rightarrow 0$  transition, which in principle should also give a contribution to the spectrum, is weighted by the proton coherent scattering length and therefore is not observed. So, for *p*- $H_2$ , only the inelastic  $J=0 \rightarrow 1$  transition contributes. In summary, each rotational transition should be followed, at higher energy, by the same spectrum  $S_{self}^{CM}(\mathbf{Q},\omega)$  of the CM excitations, apart for an intensity scaling. That this is actually the case is shown in Fig. 4. Here the plotted *p*- $H_2$  spectrum (red, panel b) is shifted to the left by 14.7 meV, that is the energy of the  $J=0 \rightarrow 1$  transition in the free molecule. In addition, the *o*- $H_2$  spectrum (black) has been plotted separating the rotational elastic contribution ( $J=1 \rightarrow 1$ ) (a) from the rotational inelastic one ( $J=1 \rightarrow 2$ ) (c). This latter has been shifted by the value of the rotational transition (29.0 meV). Now the correspondence among the different spectral bands becomes more evident. The rattling fundamental band appears at  $\approx 10$  meV to the right from each rotational transition. In addition, a visible contribution due to the first



**Figure 5.** Representation of one  $H_2$  molecule (gray dumbbell) inside the small dodecahedral cage of a clathrate. Red spheres represent oxygen atoms, while water protons are not shown. The vector  $\mathbf{R}'$  joins the two nuclei, while  $\mathbf{R}$  points from the origin to the molecule CM. The system has six degrees of freedom, and is described by the six quantum numbers  $v, J, m, N, L, M$ .

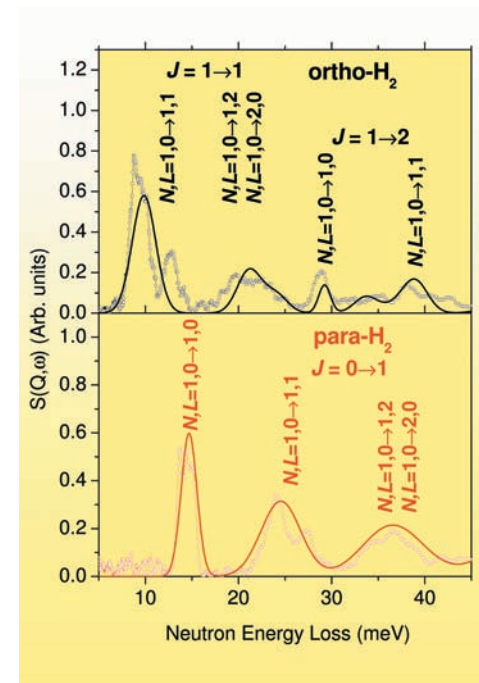
overtone of the rattling excitation appears at  $\approx 21$  meV to the right from each rotational transition energy.

A calculation of the spectral intensity of the rattling excitations, and a consequent comparison with the experimental determination, is possible, if we



**Figure 6.** Left panel: Isotropic part of the potential energy for one  $\text{H}_2$  molecule as a function of the distance  $R$  (atomic units) from the center of the dodecahedral cage, and calculated energy levels. Right panel: Calculated incoherent INS spectra for one  $\text{H}_2$  molecule (Eq. 2) (top line, blue). This is the sum of the three contributions shown below, one for each rotational transition considered, namely  $J = 1 \rightarrow 1$  and  $J = 1 \rightarrow 2$  for  $o\text{-H}_2$  (black) and  $J = 0 \rightarrow 1$  for  $p\text{-H}_2$  (red).

adopt several approximations in the calculation. We have solved numerically the Schrödinger equation for the motion of the molecular CM into the small dodecahedral clathrate cage. The coordinates that describe this motion are listed in Fig. 5, with  $\mathbf{R} = (R, \theta, \varphi)$  indicating the CM position with respect to the cage center, and  $\mathbf{R}' = (R', \theta', \varphi')$  indicating the internuclear distance and molecular orientation. Quantum-mechanically, the system is described by six quantum numbers. In the assumption of weak coupling between the CM and vibro-rotational motion, the quantum numbers retain their meaning:  $\nu, J, m$  are the intra-molecular vibrational and rotational quantum numbers, and  $N, L, M$  describe the orbital motion of the CM inside the cage. To treat the problem with elementary quantum mechanics, we have reduced the CM motion to that of one particle in a spherical potential well, by calculating the average potential energy over the directions of  $\mathbf{R}$ , (that is,  $\theta$  and  $\varphi$ ) and, in addition, over the  $\text{H}_2$  molecular orientations ( $\theta'$  and  $\varphi'$ ). The pair  $\text{H}_2\text{-D}_2\text{O}$  potential has been assumed to be equal to the  $\text{H}_2\text{-H}_2\text{O}$  potential, reported in the literature.<sup>16,17</sup> Details of the calculation are reported in ref. 9. The potential energy of the hydrogen molecule as a function of  $R = |\mathbf{R}|$ , obtained using any of the two potential models available from the literature,<sup>16,17</sup> which give the same results for the purpose of this analysis, is represented in the left panel of Fig. 6. It is strongly anharmonic: rather flat in the center and with relatively hard walls close to the cage boundaries. As a consequence, the calculated energy levels (labeled by the principal quantum number  $N = 1, 2, 3, \dots$ ), are split (the energy depends on the orbital quantum number  $L = 0, 1, 2, \dots$ ) and not equally spaced. The residual  $(2L+1)$ -fold degeneracy of each level is not removed in this model due to the assumed isotropy of the cage potential. Knowledge of the wave function for the translation degrees of freedom, and the use of Eq. (2), where



**Figure 7.** Comparison of the  $o\text{-H}_2$  and  $p\text{-H}_2$  experimental spectra with the results of our calculation, where we have considered the  $J = 1 \rightarrow 1$  and  $J = 1 \rightarrow 2$  molecular rotational transitions for the  $o\text{-H}_2$  spectrum and the  $J = 0 \rightarrow 1$  transition for the  $p\text{-H}_2$  spectrum. The assignment of some of the bands is indicated.



all coefficients  $f(J,J',Q)$  are known, enables us to calculate the intensity of the transitions, determining the whole neutron energy loss spectrum. For each rotational transition of the molecule, we obtain a spectrum given by the series of the rattling transitions energies plus the rotational transition energy. The calculated spectrum, obtained assigning the same arbitrary width to all transitions, is shown in the right panel of Fig. 6.

The comparison with experiment is done separately for *o*-H<sub>2</sub> and *p*-H<sub>2</sub> in Fig. 7. Here for each calculated transition only the width has been adjusted. We find a good level of agreement, taking into account that the aim of this simple model is to reproduce the integrated intensity of each band, but not the splitting of the bands. As a matter of fact, observing Figs. 3 and 7, we notice that both the rattling fundamental ( $\approx 10$  meV in the *o*-H<sub>2</sub> spectrum) and the  $J=0 \rightarrow 1$  rotational transition ( $\approx 14$  meV in the *p*-H<sub>2</sub> spectrum) are multiple bands composed by three component each. We remark that the splitting of the *rattling* mode depends on (and can be a measure of) the anisotropy of the potential energy with respect to the CM *position* in the cage, while the splitting of the *rotational* mode is a consequence of the anisotropy with respect to the *orientation* of the H<sub>2</sub> molecule. This issue is discussed in more detail in Ref. 9, where the comparison made with a recent calculation<sup>18</sup> indicates the need of a more precise model for the H<sub>2</sub>-H<sub>2</sub>O potential.

In summary, we have demonstrated the capability of INS to measure fine details of the quantum dynamics of a single H<sub>2</sub> molecule in the confined geometry of a water clathrate nanocavity. A simplified isotropic model describes the main features of the motion in a quantitative way, thus demonstrating that coupling between rotational and CM dynamics is weak. Frequencies and intensities of the spectrum are reproduced by this model. The splitting of the rotational and translational bands is a consequence of the anisotropy of the environment, which must be modeled with greater accuracy than done until now, to extract direct information on the basic interaction between H<sub>2</sub> and H<sub>2</sub>O.

## REFERENCES

1. E.D. Sloan, C.A. Koh, Clathrate Hydrates of Natural Gases, 3rd ed., CRC Press, Taylor and Francis, (2008).
2. Y.A. Dyadin, E.G. Larionov, A.Y. Manakov, F.V. Zhurko, E.Y. Aladko, T.V. Mikina and V.Y. Komarov, Mendeleev Commun. 9, 209 (1999).
3. W.L. Mao, H.K. Mao, A.F. Goncharov, V.V. Struzhkin, Q. Guo, J. Hu, J. Shu, R.J. Hemley, M. Somayazulu, Y. Zhao, Science 297, 2247 (2002).
4. K.A. Lokshin, Y. Zhao, D. He, W.L. Mao, H.K. Mao, R.J. Hemley, M.V. Lobanov, and M. Greenblatt, Phys. Rev. Lett. 93, 125503 (2004).
5. S. Patchovskii and J.S. Tse, Proc. Nation. Acad. Sci. 100, 14645 (2003).
6. L.J. Florusse, C.J. Peters, J. Schoonman, K.C. Hester, C.A. Koh, S.F. Dec, K.N. Marsh, E.D. Sloan, Science 306, 469 (2004).
7. K.C. Hester, T.H. Strobel, E.D. Sloan, C. Koh, A. Huq, and A.J. Schultz, J. Phys. Chem. B Lett. 110, 14024 (2006).
8. J.S. Tse, D.D. Klug, J.Y. Zhao, W. Sturhahn, E.E. Alp, J. Baumert, C. Gutt, M.R. Johnson, and W. Press, Nature Mater. 4, 917 (2005).
9. L. Ulivi, M. Celli, A. Giannasi, A.J. Ramirez-Cuesta, D.J. Bull, M. Zoppi, Phys. Rev. B 76, 161401(R) (2007).
10. L. Ulivi, M. Celli, A. Giannasi, A.J. Ramirez-Cuesta, M. Zoppi, J. Phys.: Condens. Matter 20, 104242 (2008).
11. D. Colognesi, M. Celli, F. Cilloco, R.J. Newport, S.F. Parker, V. Rossi-Albertini, F. Sacchetti, J. Tomkinson, and M. Zoppi, Appl. Phys. A: Mater. Sci. Process. A 74 (Suppl. 1), 64 (2002).
12. M. Celli, F. Cilloco, D. Colognesi, R.J. Newport, S.F. Parker, V. Rossi-Albertini, F. Sacchetti, J. Tomkinson, and M. Zoppi, Notiziario Neutroni e Luce di Sincrotrone, 6, n. 2 (2001).
13. D. Colognesi, M. Celli, and M. Zoppi, J. Chem. Phys. 120, 5657 (2004).
14. S.W. Lovesey, Theory of neutron scattering from condensed matter, Clarendon Press, Oxford, (1984), p. 24.
15. J.A. Young and J.U. Koppel, Phys. Rev. 35, A643 (1964).
16. S. Alavi, J.A. Ripmeester, and D.D. Klug, J. Chem. Phys. 124, 014704 (2006)
17. M.P. Hodges, R.J. Wheatley, G.K. Schenter, and A.H. Harvey, J. Chem. Phys. 120, 710 (2004).
18. M. Xu, Y.S. Elmatad, F. Sebastianelli, J.W. Moskowitz, and Z. Bacic, J. Phys. Chem. B Lett.

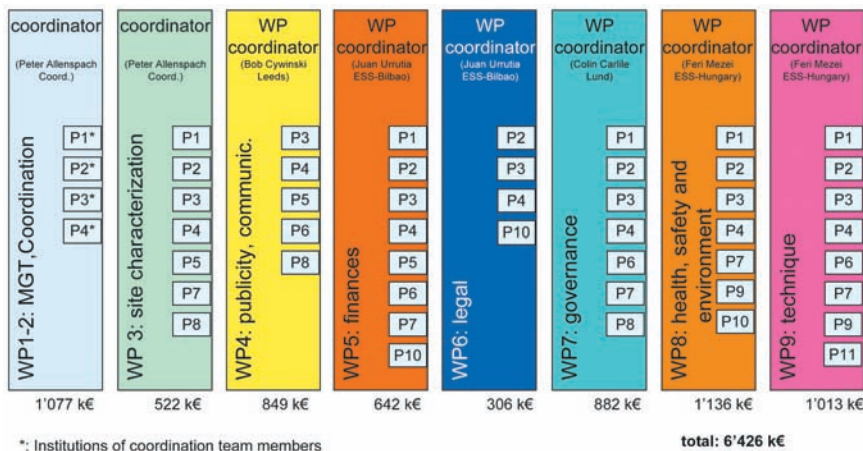


# ESS Preparatory Phase (ESS-PP)

In fall 2006 the European Strategy Forum on Research Infrastructures (ESFRI; <http://cordis.europa.eu/esfri/>) published a roadmap containing 35 mature research infrastructure projects with the European Spallation neutron Source (ESS) being one of the largest on this list. A few months later the EU launched a call for these 35 projects for preparatory work comprising legal work (legal structure of infrastructure, regulations, restrictions, licensing, intellectual property rights), governance issues (ownership policy, human resources, access framework, governing and advisory bodies), financial aspects (construction, operation, decommissioning, funding sources, fund creation), strategic issues (integration of infrastructure into EU fabric of related facilities, site issues, public relations) and some limited technical work. Our project followed this menu list and came up with the work packages shown in Fig. 1. Participants are: P1 PSI (Switzerland), P2 ESS-Bilbao (Spain), P3 Lund University (Sweden), P4 ESS-Hungary (Hungary), P5 Leeds University (UK), P6 STFC (UK), P7 FZ Juelich (Germany), P8 INFN (Italy), P9 CNISM (Italy), P10 CEA (France), P11 Latvia University (Latvia). The ESS-PP has started on April 1, 2008, and will run for two years. A huge amount of work has already been done in the past by the ESS project team and ESS is essentially ready to be built, however some additional questions have to be clarified (e.g. radioactive inventory, environmental impact, decommissioning) and some documents to be up-dated. In order not to delay any decision on ESS urgent issues will be taken on very early in the project. Recently, ESFRI launched another initiative (which will be financed via ESS-PP) in order to assess the ESS sites: The ESFRI working group on ESS siting (EWESS) sent a questionnaire to the official sites (Lund in Sweden, Bilbao in Spain and Debrecen in Hungary) which have been answered by April 25, 2008. The answers and the sites themselves will be assessed by the ESS Site Review Group (SRG) comprising 3 expert people individually accepted by all three sites. SRG will finally submit a report to EWESS on September 15, 2008. ESS-PP and EWESS/SRG actions together should facilitate a decision on the site and on ESS itself, however the decision has still to be taken on a political level.

**P. Allenspach**

ENSA chairman and coordinator of ESS-PP



**Figure.1** Work packages for ESS-PP with list of partners involved and costs foreseen.





# PETRA III: DESY's New High Brilliance Third Generation Synchrotron Radiation Source

H. Franz, R. Röhlberger, E. Weckert

Deutsches Elektronen Synchrotron, DESY, HASYLAB,  
22607 Hamburg, Germany

## ABSTRACT

DESY in Hamburg, Germany, is refurbishing the 2.3 km long storage ring PETRA into a third generation synchrotron radiation source called PETRA III. It will operate at 6 GeV particle energy, 100 mA current in top-up mode, and a horizontal emittance of 1 nmrad. PETRA III will be one of the most brilliant light sources in the hard X-ray regime with the smallest horizontal emittance worldwide. In the first phase fourteen independent undulator beamlines will be available for user experiments.

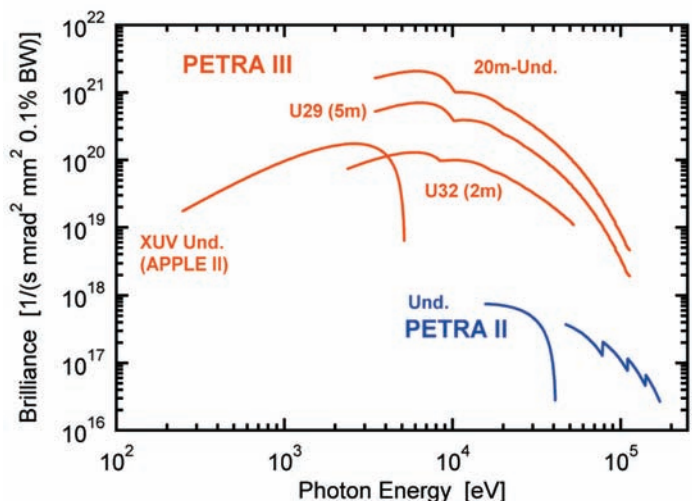
## INTRODUCTION

At present, the storage ring DORIS III (4.5 GeV, 150 mA) serves as the main source for synchrotron radiation experiments at DESY. DORIS III is a second generation storage ring with a rather large emittance of 450 nmrad, producing high flux X-ray beams of comparatively low brilliance. In order to follow the increasing user request for high brilliance beams, DESY decided to convert the storage ring PETRA into a very low emittance synchrotron radiation source called PETRA III. PETRA (positron electron tandem ring accelerator) is a storage ring with 2304 m circumference, which was built in 1976 as an  $e^+ - e^-$  collider discovering the gluon in 1978.

The main technical issues of the reconstruction and an outline of the scientific program anticipated at PETRA III have been published in a Technical Design Report in 2004 [1]. In addition to DESY the European Molecular Biology Laboratory (EMBL) and the Forschungszentrum Geesthacht (GKSS) are involved in the construction and operation of beamlines at PETRA III. The Max-Planck-Society and surrounding universities support the construction and operation of beamlines, however not dedicated to a specific technique.

## STORAGE RING

The reconstruction of PETRA includes the total rebuilding of one eighth of the storage ring. In this part the FODO lattice of the PETRA arcs will be replaced by nine double-bend achromat cells. In this way, in addition to the one existing, eight new straight sections are created. Each of them will provide space for one 5 m or two 2 m long insertion devices. The beams from the two 2 m IDs will be inclined relative to each other by 5 mrad by means of a small bending magnet installed in between the IDs. This scheme allows operating two independently tuneable undulators at a single straight section with beam paths suf-



**Figure 1.** Comparison of the brilliance of different PETRA III undulators and the former PETRA II insertion device.

ficiently separated for individual beamline optics and safety systems. The ninth straight section will be suitable for an insertion device up to 20 m in length (10 m in the first construction phase). For future upgrades there are two other positions at the PETRA storage ring where additionally up to 20 m long undulators can be placed. In addition there are three optional positions for 5 m insertion devices. In total about 19 insertion device positions will be available at the reconstructed storage ring.

The design value for the storage ring energy is 6 GeV with a stored current of 100 mA. However, all beamline and vacuum components that have to stand high heat load will be dimensioned for a current of at least 200 mA in order to have head space for further upgrades. Damping wigglers [2] with a total length of 80 m will be installed to reduce the emittance to the design value of 1 nmrad. The aim is to achieve an emittance coupling of 1 %. In order to fully benefit from this low emittance beam stability is a crucial issue. To reduce changes in heat-load and thermal drifts to a minimum, top-up operation is foreseen right from the start. Top-up operation will allow us also to offer - besides a continuous filling mode - timing mode operation with 40 equidistant bunches separated by 192 ns.

In order to ensure a reliable operation of the storage ring all magnet coils and all sextupoles of the remaining 7/8 of the storage ring will be renewed as well as the entire vacuum system. In addition, further upgrades are necessary for the storage ring's RF system, magnet power supplies, and cooling system. To guarantee sub-micron beam stability, suitable diagnostics and beam position control systems will be established. PETRA III will use the existing pre-accelerators LINAC II and DESY II. However, to ensure a very high availability of the beam in top-up mode, the injector systems will be refurbished as well.

### PHOTON BEAM PERFORMANCE

To make optimum use of the available space, we are currently focusing on ID beamlines only. Two values of the  $\beta$ -function will be available at the insertion device positions. Table 1 lists the source parameters for a standard 5 m undulator. Similar to the ESRF there will be the option to have either a low or a high  $\beta$ -value in each individual straight section. It will be possible to switch between these two  $\beta$ -function values during a short shut down period or a maintenance day.

Most insertion devices will be standard ex-vacuum undulators. Only for the

	$\beta_x$	$\beta_y$	$\Sigma_x$	$\Sigma_y$	$\Sigma_{x'}$	$\Sigma_{y'}$
	m	m	$\mu\text{m}$	$\mu\text{m}$	$\mu\text{rad}$	$\mu\text{rad}$
<b>low - <math>\beta</math></b>	1.2	4	34.5	7.3	29	5.2
<b>high - <math>\beta</math></b>	20	2.38	141	4.2	8.6	5.2

high energy beamline (starting from an X-ray energy of 50 keV) an in-vacuum undulator is foreseen. The vacuum chamber inside the standard undulators will have an internal aperture of 7 mm which results in a minimum magnetic gap of the undulators of about 9.5 mm. In Figure 1 the tuning curves of different PETRA III undulators are compared. The highest brilliance available will



**Figure 2.** View into the still empty new experimental hall.

**Table 1.** Overview of  $\beta$  functions, photon source sizes  $\Sigma_{x,y}$  and divergences  $\Sigma_{x',y'}$  for PETRA III ID positions. The photon source parameters are given for a photon energy of 12 keV and 5 m ID length. All values are rms.



be beyond  $10^{21}$  ph/(s mm<sup>2</sup> mrad<sup>2</sup> 0.1%BW) outperforming all existing sources in the range from 3 keV to 25 keV.

The standard undulator is designed to be tuneable over the whole energy range ( $K_{\max} \sim 2.2$ ). This results in a period length of  $\lambda_u = 29$  mm. In addition, there will be a “spectroscopy” undulator with 32 mm period length giving access to energies down to 2.4 keV. The abovementioned in-vacuum (IV) undulators will have a period length of 22 mm.

For photons in the VUV and XUV range, a high energy storage ring has significant advantages, if circularly polarized photons in the 250-3000 eV range are needed with a high degree of polarization, which can only be obtained on the first undulator harmonic of a helical undulator. The brilliance of such devices (e.g. a 5 m long Apple-II undulator) at PETRA III will approach the  $10^{20}$  range. It should be emphasized that the brilliance calculations above are based on the assumption of a 1 % horizontal/vertical coupling. A smaller coupling value would increase the brilliance significantly due to a smaller vertical source size. However, it will also reduce the Touschek lifetime. In general, user experiments will not benefit from this increase in brilliance since the limiting factor for most micro-focusing and coherence experiments is the horizontal emittance. The main difference in comparison with existing high energy, third generation synchrotron radiation sources, is therefore not that much in brilliance but in horizontal emittance. This results in a smaller horizontal source size and consequently a significantly larger total fraction of coherent photons or a higher number of photons accepted by any focusing optics.

In order to serve 14 beamlines with only 9 straight sections, it was decided to cant five of the straight section by 5 mrad using a short dipole magnet installed in the centre of the straight. The two insertion devices in the upstream and downstream half can be operated independently. As the distance between the two beams from these undulators is some 15 cm at the entrance of the first optics hutch, there is enough space for independent vacuum and safety systems. On the other hand this separation is not enough for bulky experiments. Thus one of these beamlines will be off-set using a so called large-offset monochromator. Details on the front-end components can be found in [3].

#### EXPERIMENTAL HALL

A new experimental hall has been built above the reconstructed eighth of the storage ring. The total area (without the space occupied by the technical infrastructure) will be approximately 9000 m<sup>2</sup>. The experimental hall is equipped with an overhead crane with a capacity of 20 tons. The experimental hall floor was cast as a single 1 m thick concrete slab on a weekend in mid December 2007. During 60 hours 6700 m<sup>3</sup> of concrete had been continuously pumped into the already closed hall. 50 % of the concrete (i.e. the upper half of the plate) is reinforced by steel fibres to ensure that the number of cracks is minimized. The slab which is one single piece of concrete will carry the ring tunnel and the experiments. It is vibrationally decoupled from the experimental hall super structure, the technical infrastructure area at the inner perimeter, and the laboratory area at the outer perimeter. To minimize the influence of the super structure on the experimental floor via coupling through the sub-soil, the super structure is founded on sleeved piles fixed 20 m deep in the ground.

The dimensions of the hall are such that beamlines can be up to 110 m long. For each beamline, laboratory space and office space is allocated on the outer perimeter of the hall. The air condition of the hall has been designed for a temperature stability of  $\pm 1\text{K}$ . Both storage ring tunnel and experimental hutches will be stabilised even better. Figure 2 shows the view into the hall as of April 2008.

Sector	Station	Methods	ID-type	Energy range keV	Responsibility
1	Dynamics	NRS, IXS	10 m U32	5 – 40	DESY
2a	SAXS/WAXS	Nano-diffraction, USAXS, micro-SAXS	2 m U29	8 – 23	DESY
2b	Hard X-ray scattering	XRD, extreme conditions	2 m U22	30 – 100	DESY
3	Variable Polarization Soft X-rays	Gas phase studies, spectro-microscopy, XRD, ARPES	5 m APPLEII	0.2 – 3	DESY
4a	Imaging, nano-tomography	Phase contrast, fluorescence tomography	2 m U29	8 – 45	GKSS
4b	Hard X-ray Microprobe	Phase contrast, fluorescence, nano-diffraction, XAFS	2 m U32	2.4 - 50	DESY
5	High Energy Materials Science	XRD, SAXS, tomography	5 m IV U19	40 - 150	GKSS, DESY
6a	High resolution diffraction	High resolution XRD, reflectivity	2 m U29	5.4 - 30	DESY
6b	Resonant X-ray Scattering	Magnetic scattering, XRD	2 m U32	2.4 - 50	DESY
7	Coherence Applications	XPCS, coherent imaging	5 m U29	4 – 25	DESY
8a	Bio-imaging, -diffraction	PX, coherent imaging	2 m U32	8 – 25	MPG, HGF, DESY
8b	BIOSAXS	SAXS	2 m U29	4 – 25	EMBL
9a	MX1	PX, MAD	2 m U29	8 – 16	EMBL
9b	MX2	micro-PX	2 m U29	4 – 35	EMBL

## EXPERIMENTAL STATIONS

The selection of the experimental stations at PETRA III was carried out in close collaboration with the user community. Starting in 2001 a series of workshops was organized to include the experience of users and experts from other facilities in the design of the experiments. An international advisory committee selected 14 beamlines out of the 22 proposed in the Technical Design Report. All of them make use of one of the special properties of PETRA III:

- coherence
- high resolution (spatial, energy, q-space)
- high energy X-rays (up to 100 keV and more)

Sector 1 will be dedicated to inelastic scattering with few meV and nuclear resonant scattering with neV energy resolution, offering simultaneously a spatial resolution in the few or even sub-micron range. Sector 2 will be shared by

**Table 2.** List of beamlines at PETRA III. Beamlines labeled by a,b denote those that share a straight section with two canted undulators (see [4] for more details).



a hard X-ray beamline with one fixed energy end-station for powder diffraction and one for extreme conditions experiments and one beamline for micro and nano SAXS applications. Sector 3 will house a variable polarization soft X-ray beamline equipped with an Apple-II type Undulator and a selection of dedicated end-stations. Sector 4 is the imaging sector with one beamline for tomography (operated by GKSS) and a hard X-ray nano-probe beamline dedicated to spatially resolved absorption spectroscopy and fluorescence analysis.

In sector 5 GKSS and DESY jointly operate a beamline for very hard X-rays (above 50 keV) dedicated mostly to materials science applications. Sector 6 focuses on diffraction experiments combining a very high resolution diffraction and a resonant scattering end station. In addition a station for electron spectroscopy will be included. Sector 7 makes special use of the high brilliance of PETRA III to perform experiments using the coherent flux. Both XPCS and coherent imaging experiments are foreseen. The last two sectors 8 and 9 are dedicated to life-science applications with four beamlines operated together with the Max-Planck society, the Helmholtz centre for infection research and with the largest part of three experiments, the European Molecular Biology Laboratory, EMBL. These beamlines will offer small angle scattering, macromolecular crystallography and bio-imaging end stations. In Table 2, the stations are listed with their main energy range and the techniques envisaged to be implemented.

### CONCLUSION

After start of operation in early 2009 PETRA III will be one of the most brilliant light source in the hard X-ray regime with the worldwide smallest horizontal emittance. Due to the size of the storage ring a number of future upgrade possibilities do exist. In addition to PETRA III the high flux hard X-ray light source DORIS III and the VUV free electron laser FLASH are available for user experiments at DESY. In this collection of light sources PETRA III will provide high brilliance X-ray beams with the superior stability storage ring sources can provide. The insertion devices will cover an energy range from the VUV (200 eV) up to very hard X-rays (150 keV). In particular all experiments making use of the small source size and simultaneous low divergence will gain considerably compared to any existing source.

### ACKNOWLEDGEMENTS

We thank all our colleagues from DESY and other SR laboratories as well as all workshop participants who have contributed to the project.

### REFERENCES

1. K. Balewski, W. Brefeld, W. Decking, H. Franz, R. Röhlberger, E. Weckert, PETRA III: A low emittance Synchrotron Radiation Source, DESY internal report 2004-035, 2004
2. H. Wiedemann, An ultra-low emittance mode for PEP using damping wigglers, Nucl.Inst.Meth.A 266, 24 (1988)
3. U. Hahn, H.B. Peters, R. Röhlberger, H. Schulte-Schrepping, The Generic Beamline Concept of the New PETRA III Undulator Beamlines, in "Proceedings of the SRI-2006", 2006
4. <http://petra3.desy.de>



# An Upgrade for the European Synchrotron Radiation Facility

In order to maintain its leading role and to respond to the emerging scientific challenges, the ESRF is planning an ambitious Upgrade Programme, comprising (i) the extension of the experimental hall to enable the construction of new and upgraded beamlines with largely improved performance and new scientific opportunities, as well as improved infrastructures for the preparation of experiments, (ii) a programme of improvements of the accelerator complex, (iii) a strong supporting programme of engineering and technology developments, and (iv) the development of productive science and technology driven partnerships. The planned Upgrade will enable significant progress in fields such as nanoscience and nanotechnology, structural and functional biology, health, environment, energy and transport, information technology, and materials engineering. The Science case and the related technological challenges are laid out in an exhaustive document, the so-called Purple Book, which has been already widely disseminated, and is available on the ESRF website ([www.esrf.fr/AboutUs/Upgrade/purple-book/](http://www.esrf.fr/AboutUs/Upgrade/purple-book/)).

The enhanced experimental facilities, in conjunction with intense efforts towards an integrated approach using synchrotron and laboratory-based techniques, promise major impact in information and communication technologies, health and environment, as well as cultural heritage. To cite several of the most prominent examples: (1) The provision of nanometre scaled X-ray beams will help reveal the relation between structure, magnetism and function of quantum confinement-induced properties of nanoscale materials, crucially required for novel (opto)-electronic and magnetic storage media. (2) Three-dimensional sub-micrometre and nano-tomographic imaging and spectroscopy tools will allow the location and role of metals in biology and medicine to be addressed, in particular in connection with neurodegenerative diseases and cancer treatments. (3) massive-throughput macromolecular crystallography facilities will face the key tasks of the pharmaceutical industry – generation of new drugs, where an essential aspect of this endeavour is the screening and analysis of thousands of compounds. (4) The multiscale investigation of in-situ growth/failure of materials, behaviour of porous (rocks) or granular materials and storage materials for solar and hydrogen energy as well as nuclear waste will be essential to enable new technologies aiming at preserving our planet and our quality of life.

The 10-year Upgrade Programme sets out the plans for 287 M€ (in 2008 prices) of expenditure resourced from 201 M€ of new Members' contributions (corresponding to an annual share of 20 M€ over the programme), from 9 M€ of Scientific Associates' contributions and from 77 M€ of the "regular" ESRF budget. This includes the option for a joint high magnetic field laboratory with ILL and other key high field European laboratories, estimated at 35 M€ in total (capital = 25 M€ and operating costs = 10 M€). In its current stage the programme consists of two phases, each with options. Funds of 4.99 M€ have

M. Krisch



**Figure 1.** Artist's impression of the planned extension of the current ESRF experimental hall and the common ESRF-EMBL-ILL site.





been granted by the European Commission within the FP7 Capacities Programme (Acronym ESRFUP) in September 2007. These funds are of critical importance in the preparation of the ESRF Upgrade in its various aspects, particularly in catalysing and strengthening the science cases for the new beamlines with the involvement of the user communities. Over the coming year, conceptual design reports for the new beamlines will be drafted and the updated floor plan of the ESRF experimental hall prepared and presented to the ESRF Science Advisory committee. The extended experimental hall is expected to be completed for the start of 2012 when the new, long beamlines can start construction.

The planned Upgrade has been presented and intensively discussed with the ESRF's user community, the advisory committees and the governing body of the ESRF, the Council. The ESRF Council and Directors have undertaken individual discussions with high-level representatives of all 18 member countries, and have received strong support. It is expected that Council will make a firm financial commitment in June 2008.

## New Head of Users' Office at ESRF

*M. Capellas*

One of the main correspondents to the users is the Head of the Users' Office. The former head, Roselyn Mason, began in the job when the office was first created. Since her retirement in April, Joanne McCarthy is leading the group. This British physicist was until now the beamline operations manager in the Macromolecular Crystallography group. Her experience as a scientist, as well as in dealing with the administration associated with the user programme of the MX beamlines, has given her good grounds on which to start her new job.

Joanne McCarthy (right) with her team  
(top from left to right: Nadine Petricola, Agnès Carlet; below: Sonya Girodon).  
[Credits: Chantal Argoud]

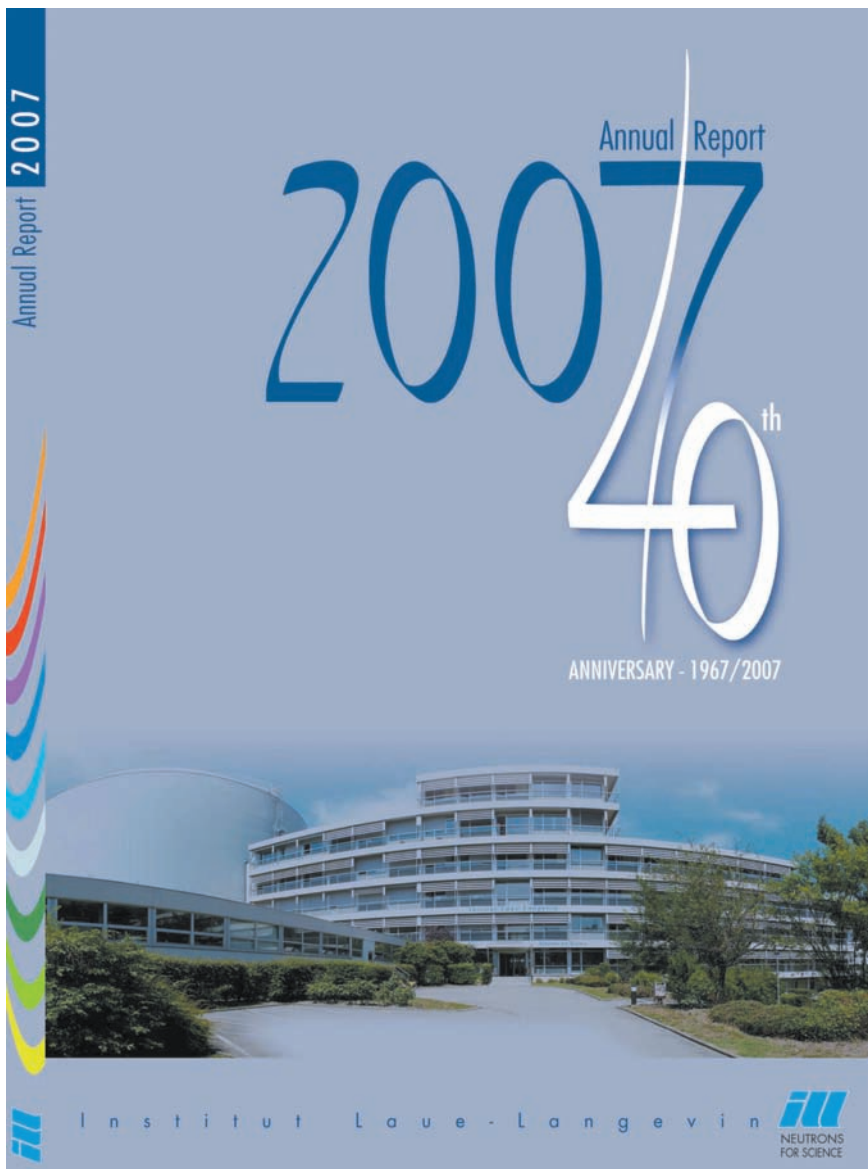




# News from the user office

## ANNUAL REPORT 2007

The ILL Annual Report 2007 has been published! It is also available on a CD ROM, which contains the pdf files of the ILL Experimental Reports 2007 and an interactive virtual visit of the ILL as well. Please get in touch with us if you want a copy of our Annual Report ([sco@ill.fr](mailto:sco@ill.fr)). Alternatively, you can find an electronic version on the ILL web-site ([www.ill.fr](http://www.ill.fr), Publications, Annual Report). Please note that the dead line for sending your contribution to the next Annual Report is 1 October 2008.





#### LONG TERM PROPOSAL SCHEME

The ILL is establishing a Long-Term Proposal (LTP) scheme similar to the one already operating at the ESRF (cfr. ILL News, December 2007, [www.ill.eu/top-links/publications/ill-news/](http://www.ill.eu/top-links/publications/ill-news/)). The ILL Scientific Council and the ILL management believe that LTPs could be beneficial to the ILL community as a whole, and we have therefore decided to give it a try. The LTP scheme will be introduced for the first time at the next proposal deadline (16 September).

#### HOW WILL IT WORK?

LTPs will be granted to ILL users for projects that extend over several cycles if it can be demonstrated that they bring extra resources or capabilities that are of benefit to users in general. About 10% of the total available beamtime will be allocated to LTPs. Users may request a long-term commitment from the ILL to provide beamtime during up to six successive scheduling periods (three years) without re-submission of new proposals. Scientific excellence is the primary criterion for the acceptance of such a Long-Term Proposal (LTP). Further criteria are:

- a commitment from the proposing User group concerning the contribution of financial, technical and/or human resources during the implementation of the LTP;
- an identifiable benefit to the ILL User community (such as a new technique, a new instrument or new possibilities for the instrument) expected to result from the successful accomplishment of the goals for the LTP.

Each LTP must be identified with a spokesperson. The spokesperson should be affiliated to a scientific institution of an ILL member country.

The implementation of a LTP requires yearly reports and a final report. In case of failure to submit a yearly report, the ILL Management reserves the right to stop the allocation of beamtime to the User group operating the LTP. Failure to submit a final report may affect the acceptance of future LTPs and beamtime proposals submitted by members of the User group concerned. LTPs can be submitted once a year. Beamtime for accepted LTPs becomes available during the following scheduling period, i.e. the third and fourth cycles of the year.

For the submission of a LTP the specific LTP application form must be used.

#### **NEXT STANDARD PROPOSAL ROUND: CALL FOR PROPOSALS**

The deadline for proposal submission is Tuesday, 16 September 2008, midnight (European time) Proposal submission is only possible electronically. Electronic Proposal Submission (EPS) is possible via our Visitors Club (<http://club.ill.eu/cv/>), once you have logged in with your personal username and password.

The detailed guide-lines for the submission of a proposal at the ILL can be found on the ILL web site: [www.ill.eu/users/proposal-submission/](http://www.ill.eu/users/proposal-submission/).

The web system will be operational from 1 July 2008. Please allow sufficient time for any unforeseen computing hitches. You will receive full support from the Visitors Club team. If you have any difficulties at all, please contact our web-support ([club@ill.eu](mailto:club@ill.eu)).



For any further queries, please contact the Scientific Coordination Office (sco@ill.eu, [www.ill.fr/users/information/user-support2/](http://www.ill.fr/users/information/user-support2/)).

### INSTRUMENTS AVAILABLE

The following instruments will be available for the forthcoming round:

- powder diffractometers: D1A, D1B\*, D2B, D20, SALSA
- liquids diffractometer: D4
- polarised neutron diffractometers: D3, D23\*
- single-crystal diffractometers: D9, D10, D15\*, VIVALDI
- large scale structure diffractometers: D19, DB21, LADI
- small-angle scattering: D11, D22
- reflectometers: ADAM\*, D17, FIGARO
- small momentum-transfer diffractometer: D16
- diffuse-scattering spectrometer: D7
- three-axis spectrometers: IN1, IN8, IN12\*, IN14, IN20, IN22\*
- time-of-flight spectrometers: IN4, IN5, IN6, BRISP\*
- backscattering and spin-echo spectrometers: IN10, IN11, IN13\*, IN15, IN16
- nuclear-physics instruments: PN1, PN3
- fundamental-physics instruments: PF1B, PF2, S18\*

\* Instruments marked with an asterisk are CRG instruments, where a smaller amount of beamtime is available than on ILL-funded instruments, but we encourage applications for these. You will find details of the instruments on the web <http://www.ill.fr/instruments-support/instruments-groups/>



### SCHEDULING PERIOD

Those proposals accepted at the next round in March will be scheduled during the first two cycles in 2009.

Cycle	Start	Shutdown
091 (or 154)	31 March	20 May
092 (or 155)	03 June	23 July
093 (or 156)	26 August	15 October
094 (or 157)	29 October	18 December

### REACTOR CYCLES FOR 2009 (PROVISIONAL)

Start-ups and shut downs are planned at 8:30 am





# Renaissance of the IN5 time-of-flight spectrometer

J. Ollivier, L. Didier, H. Mutka  
ILL, on behalf of the IN5 project team

The year 2007 has seen the completion of key parts of the IN5 new secondary spectrometer. The manufacture and tests of the position sensitive detector (PSD) panels have been completed and the time-of-flight vacuum chamber that will host the detectors has been delivered to the ILL. Pre-assembling and various tests will now run up to the installation at the instrument position by early 2008.

The IN5 high-precision direct-geometry spectrometer located on the H16 cold neutron guide has been undergoing upgrading for almost 10 years. Following the primary spectrometer (neutron guide and disk chopper) completed at the end of 2002, the secondary spectrometer (from the sample to the detectors) will mark a new milestone in the life of this 30 year old instrument.

The primary spectrometer upgrade gave a notable increase of the neutron flux at the sample, enlarged the accessible resolution range and improved the reliability of the instrument. The new secondary spectrometer promises a breakthrough in the cold neutron time-of-flight technique. Combined with the increase of the effective detection solid angle, the qualitative novelty will be a position sensitive detector (PSD) array in a vacuum time-of-flight chamber. This improvement in detection aims at allowing single crystal studies in addition to conventional spectroscopy.

## THE SECONDARY SPECTROMETER

PSD technology has already been applied on time-of-flight instruments. Nevertheless, that improve the transition between the 2 sentences is missing. This will allow probing of the high-resolution energy range covered by cold neutrons complementing the thermal instruments using PSDs.

Progress in detection electronics has relaxed the constraints on the detector length. The required spatial resolution on IN5 will be achieved with 3 metre-length detectors. An array made of such long tubes modifies the shape of the detector assembly which is now no longer tangent to a sphere but cylinder-shaped. Despite some disadvantages, the cylindrical shape allows simplifications of the design of the secondary spectrometer, e.g. detector mounting.

## THE POSITION SENSITIVE DETECTORS

The PSDs will cover the inner back surface the chamber 4 m from the sample (see figures 1 and 2). The total detection area will be six times larger than before and will boost the neutron count-rate by the same amount.

32 detector tubes are grouped in a single panel defining a detector unit sharing the same volume of gas. This unique design has been patented by the ILL Detector Group. Positioning of the units in the flight chamber has been optimised for minimal distances between panels in order to maximise the effective detector area and to avoid gaps in the experimental spectra.

The gas pressure results in 80% detection efficiency at IN5's maximum flux.

Such efficiency is suitable for the needs of low-energy scattering, limiting the quantity of  $^3\text{He}$  to be used. The low pressure also allows the thickness of the tube walls to be reduced to a minimum without compromising on security. Design and manufacturing of the PSDs have been realised in-house by the ILL Detector Group with the help of a subcontractor. Production of the 13 units (12 in operation and one spare) has taken a full year and was finished at the end of June 2007.

#### THE TIME-OF-FLIGHT CHAMBER

In order to obtain a seamless and homogeneous detector surface from scattering angles as low as  $2^\circ$  to up to  $140^\circ$ , the chamber is designed to withstand a primary vacuum. The massive vacuum-tight chamber is made of aluminium giving a fully nonmagnetic environment around the sample area.

The large detector solid angle as seen from the sample, is the reason for the absence of a window between the sample and the flight chamber. This should not interfere with the frequent changes of sample environment on IN5 (cryostats, furnaces, magnets...) since, with a properly designed pumping system, the nominal vacuum can be achieved in less than 2 hours despite the large volume to evacuate. Manufacturing of the chamber by a British subcontractor near Cambridge took nearly 15 months, under the tight control of the ILL design office.

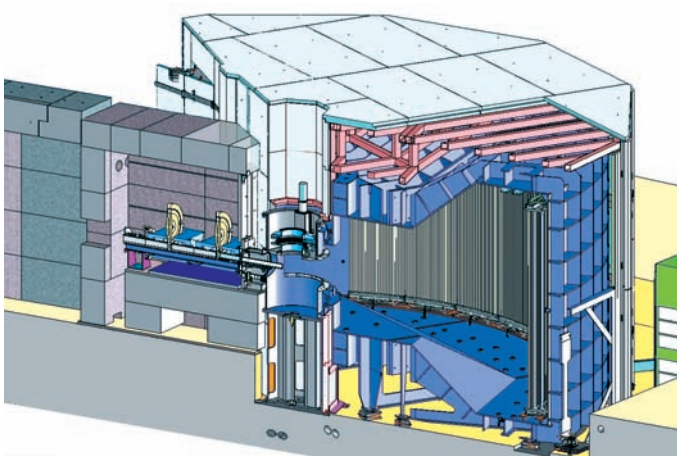
#### THE BACKGROUND PROTECTION (DETECTOR SHIELDING)

In order for the combination of the detectors and flight chamber to perform appropriately the neutron background must be as low as possible.

According to previous measurements, within the available space, weight and cost limitations, a layered structure made of a high-density polyethylene neutron moderator, with an inner surface lining of 5 mm of B<sub>4</sub>C - charged polyurethane was installed in spring 2006 (see figure 3). The new shielding that encloses the present unitary detectors has reduced the background by an estimated factor of four when compared to the former shielding. A comparison with the neighbouring IN6 instrument as well as with the new time-of-flight TOFTOF in Munich has shown that IN5 achieves a similar signal-to-noise ratio as these instruments.

**Figure 1.** Vertical slice along the beam axis showing the last choppers, the sample chamber, detector array, flight chamber and detector shielding [Image courtesy of B. Grenappin].

**Figure 2.** Three detector units mounted inside the time-of-flight chamber. The inner chamber height at detector position is 3.5 m; the detector unit full height is 3.2 m.





### THE FIRST MILESTONE: THE TEMPORARY SECONDARY SPECTROMETER

A first milestone was the reopening of the instrument to users after replacement of the detector shielding and the digging of a recess in the floor in order to accept the new larger flight chamber. It was also necessary to reinforce the floor because of the weight of the new secondary spectrometer. This operation did not affect scheduled users since all the work was carried out during the long shutdown required for the ILL refit programme.

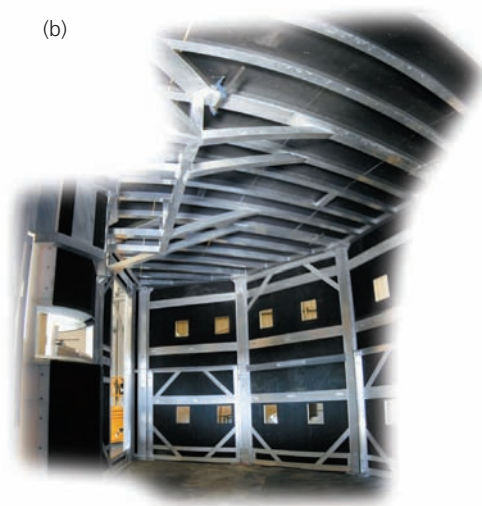
### INSTALLATION, COMMISSIONING AND FUTURE

Started in 2004, the secondary spectrometer project is expected to be completed before commissioning of the new instrument during the second reactor cycle of 2008. 2008 will see the renaissance of IN5, which started with the primary spectrometer project 10 years ago.

The new IN5 will have nothing in common with the former 30 year old instrument, opening up new fields of physics. Indeed, in addition to the new detectors, every effort has been made to allow the installation of a wide range of sample environments. The nonmagnetic chambers will allow high magnetic fields. A specific compensated coil with an asymmetric opening in order to cover a maximum detector area is to be developed in the future.

Furthermore, the size of the sample chamber will enable a polarisation device ( $^3\text{He}$  polariser, flippers and XYZ coils) to be installed. A beam polariser and a hyper-focusing nose guide for concentrating the beam on tiny single crystals have already been foreseen.

**Figure 3.** IN5 with its new neutron shielding as seen from above. (a) the inside of the protection shows the aluminium frame and the neutron absorber (b) the windows will allow direct access to the detector main electronics that will be mounted on the back of the flight chamber.



(b)

(a)



# International Conference on Neutron Scattering (ICNS)

**will be in Knoxville, TN (USA) in May 2009**

The 2009 International Conference on Neutron Scattering will be held in Knoxville, TN, USA, during May 3-7, 2009. Held under the auspices of the Neutron Scattering Society of America, this meeting follows the highly successful ICNS2005 in Sydney, Australia. An International Advisory Committee is being formed and committees responsible for the program, publications, and local arrangements will be announced soon. The workshop website is <http://neutrons.ornl.gov/conf/icns2009>. Please send your suggestions about workshop content to [ICNS2009@ornl.gov](mailto:ICNS2009@ornl.gov). Participants at the ICNS meeting will have the opportunity to tour neutron scattering facilities at Oak Ridge National Laboratory—the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR).

In the fiscal year beginning in October 2007, the HFIR was scheduled for six cycles with an anticipated >90% reliability. The fourth HFIR cycle this fiscal year (the seventh since the restart of the reactor one year ago with a new cold source) was recently completed and availability to date is 100%. Three additional instruments are anticipated to join the general user program beginning in September 2008: the Neutron Powder Diffractometer (HB-2A), the US-Japan Wide-Angle Neutron Diffractometer (WAND, HB-2C), and the Single-Crystal Four-Circle Diffractometer (HB-3A), giving a total of nine HFIR instruments in the user program.

The Spallation Neutron Source continues its power increase towards the goal of 1.4-MW. In April 2008, the SNS is operating at 400kW. In February 2008, the SNS was recognized for a Guinness World Record as the “World’s most powerful pulsed spallation neutron source.” Beam power is planned to peak at 750kW at the end of the run cycle ending in July 2008. As part of the continued enhancement of sample environment capabilities, a new shielded asymmetric magnet system has been received. It produces a central field of up to 5 tesla (T) with the advantages of very low stray field (less than 0.0005 T at 50 cm from the sample), an asymmetric field profile optimized for using polarized neutron beams, and a compact size.

Three new SNS instruments are expected to enter the general user program in the run cycle beginning in September 2008. The Wide Angular-Range Chopper Spectrometer (ARCS, BL-18) is optimized to provide a high neutron flux at the sample and a large solid angle of detector coverage and its capabilities were described in an article in *Notiziario*, volume 13 (1). The Spallation Neutrons and Pressure Diffractometer (SNAP, BL-3) allows studies of a variety of powdered and single-crystal samples under extreme conditions of pressure and temperature. The Cold Neutron Chopper Spectrometer (CNCS, BL-5) opened its shutters and received its first neutrons on April 2, 2008; it is a high resolution, direct geometry, multi-chopper inelastic spectrometer designed to provide flexibility in the choice of energy resolution and to perform best at low incident energies (2-50 meV).

**A. Ekkebus**

OAK Ridge National Laboratory, TN, USA





The proposal call in January 2008 for the experimental period April-August 2008 resulted in the receipt of about 250 proposals. The instruments at both the SNS and HFIR are in high demand from the user community, with requests for beam time approximately three times greater than that available.

#### **FIRST SCIENCE RESULTS AT SNS**

SNS instruments have already reported scientific results. In a paper accepted by *Journal of Physics*, G. Ehlers and colleagues studied the evolution of the structural properties as well as the static and dynamic spin correlations of spin ice  $\text{Ho}_2\text{Ti}_2\text{O}_7$ , where Ho was partially replaced by nonmagnetic La. Structural characterizations were done by x-ray and neutron diffraction and by Ho L-III-edge and Ti K-edge extended x-ray absorption fine structure (EXAFS) measurements. Quasielastic neutron scattering experiments were performed at NIST's DCS spectrometer and at the new Backscattering Spectrometer (BL-2) at the SNS. The experiments showed that above the macroscopic freezing temperature (1 K), the spin-spin correlations are short ranged and dynamic in nature. The main difference to pure spin ice in the dynamics is the appearance of a second, faster, relaxation process.

The March 28, 2008 issue of *Physical Review Letters* [E. Kharlampieva, et al., *Phys. Rev. Lett.* **100**, 128303 (2008)] contained the first paper published based on research at the SNS. E. Kharlampieva and colleagues used the Liquids Reflectometer (BL-4B) to study the ordering of pH-responsive polyelectrolyte multilayers. These layers represent a new class of nanostructured materials obtained through alternating assembly of water-soluble polymers at solid-liquid interfaces. The sensitivity of these films to environmental stimuli, such as pH, is useful in applications such as drug delivery, control of electroosmotic flow in microchannels, fabrication of metal-containing inorganic nanocomposite materials, and preparation of controlled porosity anti-reflective coatings.

#### **SCIENCE HIGHLIGHTS FROM HFIR**

Two separate papers submitted for publication reported recent studies of the new class of iron based layered superconductors performed at the HFIR. McGuire et al. (cond-mat/0804.0796) and de la Cruz et al. (cond-mat/0804.0795) reported the first neutron scattering observations of the spin density wave in  $\text{LaFeAsO}$ . These authors reported that doping this material with fluorine results in the suppression of the magnetic ordering at the same time that superconductivity sets in, which is reminiscent to the appearance of superconductivity in the high  $T_c$  cuprates near the concentration where magnetic order occurs. The work of de la Cruz et al. at HFIR complements measurements performed at the NIST reactor.

#### **EDUCATION WORKSHOP**

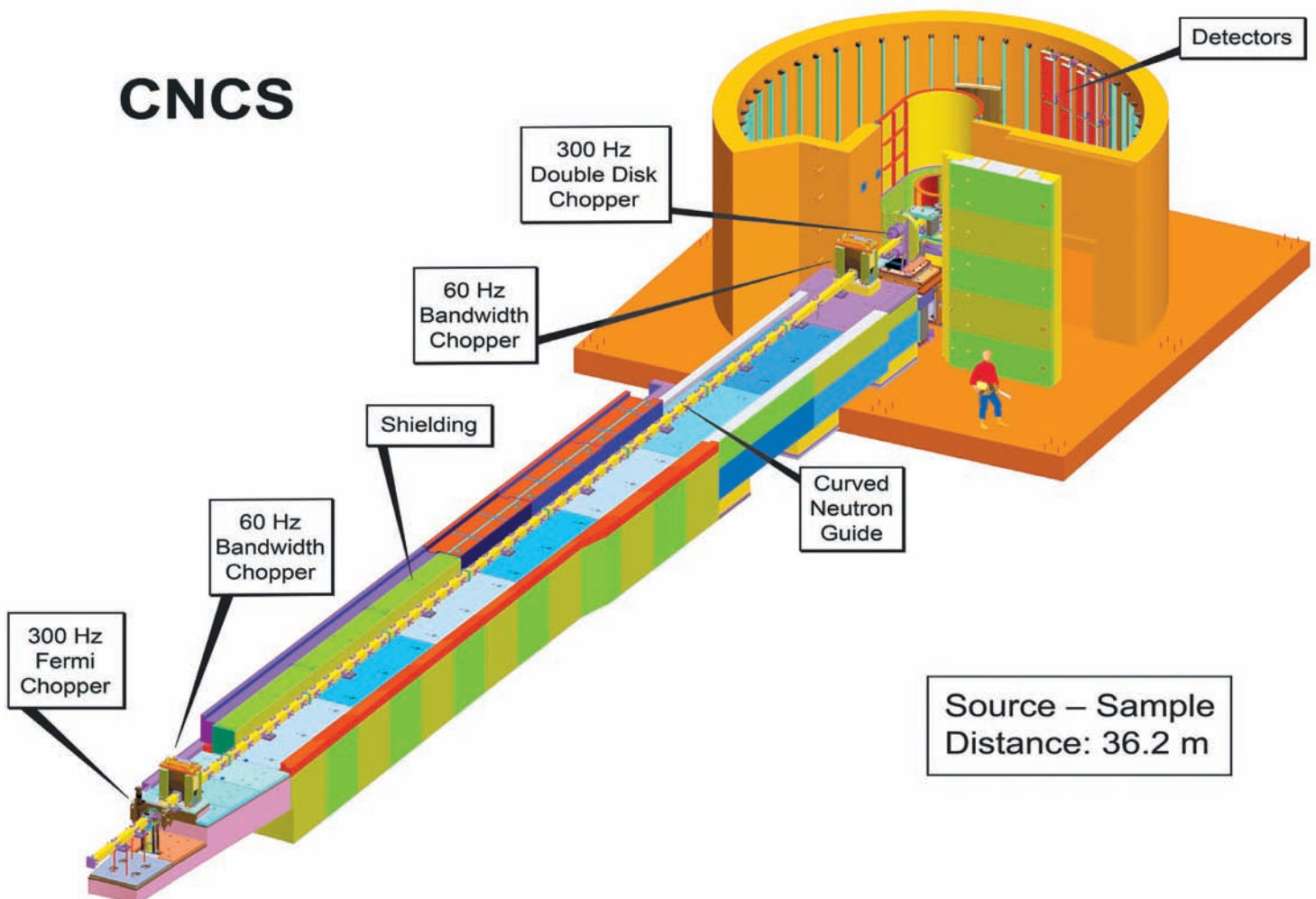
Defining a roadmap for a comprehensive neutron scattering education program in the U.S. was the goal of workshop held in suburban Washington, D.C., March 27-28, 2008. The 45 mainly U.S. attendees with observers from the international community identified best practices in providing education about capabilities of neutron scattering and in ensuring participation from a broad commu-



nity both in terms of range of scientific fields and underrepresented groups. One of the Workshop's recommendations involved creation of a web site to be called "neutronsources.org" that would be similar in function to the existing "lightsources.org" which coordinates information about x-ray synchrotron sources. There are many opportunities for this to become a portal to several proposed web-based educational activities. This new web site might include a wiki or bulletin board to support conversations about multiple aspects of neutron scattering such as data analysis or instrumentation. A neutron-pedia might provide hyper-linked information (such as the ILL Neutron Data Booklet) about neutron scattering to a scientifically literate audience. Potentially, this web site might also include a database of teaching material, such as lecture notes, downloadable video lectures and podcasts, that would be well-indexed and available for use across institutions. Of benefit to both prospective and experienced users would be the inclusion of a "neutron path-finder" (similar to that at the European Neutron-Muon Portal) to enable prospective users to identify the suitable instrument for their experiments. Information on the capabilities of the instruments mentioned previously is at <http://neutrons.ornl.gov>

The Cold Neutron Chopper Spectrometer is on SNS Beam Line 5.

## CNCS





# NEUWAVE1

## NEUtron WAVElength-dependent Imaging

### International Workshop on Energy selective neutron imaging

was successfully held  
in Munich-Garching  
from April 20th to 24th, 2008

For the first time, a meeting was held outside the “normal” sequence of conferences in neutron imaging for a dedicated topic gaining such high interest and participation. During 3 and 1/2 days, about 40 leading experts from 9 countries all over the world exchanged their knowledge about two promising topics: Energy-dependent Imaging with cold neutrons and the progress in fast neutron imaging. A new format was successfully applied for the first time, with the number of talks very limited but with plenty of time for vivid discussion.

The FRM II research neutron source “Maier-Leibnitz” of Technische Universität München was chosen as conference site due to its expertise in both fields with its facilities ANTARES (cold neutron imaging) and NECTAR (fast neutron imaging). This activity was supported by the European network NMI3 ([http://neutron.neutron-eu.net/n\\_nmi3](http://neutron.neutron-eu.net/n_nmi3)).

During this meeting it became obvious that the new approach to do also transmission imaging measurements with narrow energy bands of the applied neutron spectrum will enable a new field of material research and material characterization with cold neutrons. Because the number of facilities presently available for such kind of studies is very limited (about 5 worldwide), the presented results are only preliminary, but very promising.

It was demonstrated that the scattering behavior of most metallic materials for cold neutrons is characterized by the Bragg edges in the cross-section data due to the determined reflections at the lattices of the micro-crystallites. Depending on the neutron wavelength and the material properties, either the structural parameter of the material can be derived from transmission data, or local textures can be visualized in high spatial resolution. First impressive results of such imaging studies were presented.

These findings have direct impact on the decisions to go ahead to install also beam lines for neutron imaging at the upcoming new spallation neutron sources (ISIS-TS2, SNS, J-PARC, ESS-S). The pulse structure at these strong neutron sources is extremely promising for energy selective imaging, using the Time Of Flight (TOF) technique with high performance in respect to energy resolution and pulse intensity. The intense pulses can also be used for stroboscopic imaging of fast processes. Currently, all four sources are on different levels of consideration in respect to the installation of imaging facilities.

At ISIS-Target Station 2 (TS2), a project named IMAT is on the way for material research applications as extension and complement to activities at ENGINE-X. The goal is a setup which combines the imaging capability with a diffraction device for texture and stress analysis.

SNS is on a good way to reach the power of ISIS soon and will go beyond. Therefore, a real competition for the remaining beam ports at this source is expected. It will be necessary to apply for such a beam line option at the meeting of the Scientific Committee foreseen to be held in October 2008 with a Letter of Intent. A combination with a scattering device, e.g. a miniaturized SANS, was

considered, which would strengthen the scientific impact of the proposal. J-PARC will start operation during 2008 and commence user operation at the end of the year. The proposal system will start in Summer 2008. An elaborate universal test beam line is about to be completed for the start of user operation, which incorporates nearly all installments necessary for neutron imaging. Test measurements for imaging will be performed soon after commissioning in order to make a forecast for the future performance of a dedicated installation and to underline the layout design with realistic data.

ESS will have (if agreed) a strong intended link to industry, where neutron imaging will certainly play an important role. Although it is too early to make direct considerations in respect to design and layout of such an installation, ESS can take profit from the progress and the experience at the other sources mentioned above.

Beside these very important considerations about the future imaging capabilities at pulsed spallation sources, interesting new results in neutron imaging were presented. This was in particular about imaging with polarized neutrons for magnetic field and structure determination, phase contrast imaging, new set-up for fuel cell research and options for high resolution neutron imaging detectors. It became also clear that imaging and scattering methods will be more and more integrated and combined in future experiments.

The meeting was concluded with the explicit aim of the participants to continue the approaches and discussion in a follow-up event (NEUWAVE 2) to be held at one of the four sites of the pulsed spallation sources. The final decision about site, timing and content will be taken by latest at the ITMNR-6 meeting in Kobe (Japan), September 2008, (<http://www.org.kobe-u.ac.jp/itmnr-6/>).



Group photo of participants to the International Workshop NEUWAVE1

## New opportunities and challenges for liquid and amorphous materials science

which will take place at the ESRF, Grenoble, France on 3-4-5 September 2008

This workshop aims to highlight new horizons in the field of liquid and amorphous materials, with special emphasis on those which can be tackled with Synchrotron radiation and Neutrons related methods.

Topics will include nucleation and glass formation, dynamics at THz frequencies, interfacial phenomena, warm dense matter, dynamical heterogeneities, metallic systems. The evolutionary lineage, state of the art and future developments of related methodologies will be presented: Modern EXAFS and Diffraction, Inelastic Scattering of X-rays and Neutrons, Time resolved Pump and Probe experiments, ab initio numerical studies.

Special attention will be devoted to science at extreme conditions and related setups: levitation, laser melting, high pressure and temperature conditions.

The workshop is open to all those interested. All participants are encouraged to contribute a poster or an oral presentation to this event.

You will find more information and the electronic registration form on our web site: [www.esrf.fr/events/conferences/noclams](http://www.esrf.fr/events/conferences/noclams) A preliminary programme will soon be available.

On behalf of the Organising Committee  
**G. Monaco** (ESRF)  
**T. Scopigno** (CNR INFN)





# EMAS 2008 - The 8<sup>th</sup> Regional Workshop of the European Microbeam Analysis Society

## MEETING REPORT

The 8<sup>th</sup> Regional Workshop of the European Microbeam Analysis Society (EMAS), took place in Trieste, at the Abdus Salam International Centre for Theoretical Physics (ICTP), on April 19-22, 2008.

With the participation of some 60 scientists from 15 different European Countries this edition of the Workshop focussed on the latest developments in a wide variety of microbeam techniques spanning from electron microscopy techniques to the use of focussed photon beams from Synchrotron sources. This latter aspect represented a most welcome novelty in this series of workshops, traditionally devoted to the tutorial aspects of electron and ion beam analytical techniques and applications to all fields of material science and especially aimed at young scientists approaching this field of interest from a large variety of perspectives.

Subjects dealt with in the tutorial sessions included: theory and practice in quantitative microanalysis in the SEM and EPMA (EDS and WDS); light element analysis; Monte Carlo simulation; analytical modes in the TEM (EDS and EELS); analytical procedures in accelerator-based microscopy and spectroscopy (EXAFS, XANES), including phase contrast tomography and imaging with highly penetrating probes such as high energy photons, neutrons and free electron lasers.

Applications included studies on a large variety of materials from thin films to minerals, biological tissues, cultural heritage materials and artefacts, food

Group photo of participants to the 8<sup>th</sup> Regional Workshop of the European Microbeam Analysis Society (EMAS) in Grignano-Miramare, Trieste, Italy.





structure and properties, nuclear waste and forensic materials, cometary particles, etc. The round table discussions and poster sessions provided ample opportunity for an informal and profitable exchange among the participants, eager to share their experiences and needs, from the leading expert to the near-novice level.

The Workshop's traditionally compact format favoured cross fertilization of ideas between the two worlds of conventional and non-conventional microscopies the latter being represented by the latest developments at third generation synchrotron light sources, strongly favoured in this case by the close association between the ICTP, Elettra, the Italian synchrotron in Trieste and its newly developed free electron laser lab, Fermi@Elettra. A visit to the synchrotron facility and the newly developed lines for microscopy, microdiffraction and microanalysis closed a most profitable meeting. Selected scientific papers from works presented at the meeting will be published in *Microscopy and Microanalysis*.

The local Organizing Committee: Gabriele Tamborini of ITU, Karlsruhe, Claudio Tuniz of ICTP, Trieste (co-chairmen), Romano Rinaldi of EMAS Board and University of Perugia and Christine Walther of ITU, Karlsruhe, wish to express their gratitude to ICTP and UNESCO, Sincrotrone Trieste SCpA, the JRC of the European Commission, the IAEA and EMAS for a scientifically very profitable Workshop.

## 10th National School on Neutron and X-ray Scattering

September 24 - October 11, 2008

at Argonne National Laboratory, Argonne, IL and Oak Ridge National Laboratory, Oak Ridge, TN

### Purpose

The main purpose of the National School on Neutron and X-ray Scattering is to educate graduate students on the utilization of major neutron and X-ray facilities.

Lectures, presented by researchers from academia, industry, and national laboratories, will include basic tutorials on the principles of scattering theory and the characteristics of the sources, as well as seminars on the application of scattering methods to a variety of scientific subjects. Students will conduct four short experiments at Argonne's Advanced Photon Source and Oak Ridge's Spallation Neutron Source and High Flux Isotope Reactor facilities to provide hands-on experience for using neutron and synchrotron sources.

### Target Audience

Graduate students attending U.S. universities majoring in physics, chemistry, materials science, or related fields.

**Email address:** [nxschool@dep.anl.gov](mailto:nxschool@dep.anl.gov)

**Application Deadline: June 26, 2008**

### How to Apply

*Applicants are encouraged to register electronically through the Argonne Division of Educational Programs website at [www.dep.anl.gov/nx](http://www.dep.anl.gov/nx). Applicants not having internet access may request an application form by contacting:*

**Neutron and X-ray School  
Division of Educational Programs  
Argonne National Laboratory  
9700 S. Cass Avenue, Bldg. 223  
Argonne, IL 60439**

**Phone: 630-252-4114  
Fax: 630-252-3193**

Please visit website at [www.dep.anl.gov/nx](http://www.dep.anl.gov/nx) for more information



# Call for Proposal [Deadlines for proposal submission]

## Neutron Sources

<http://pathfinder.neutron-eu.net/idb/access>

**15th September 2008** **BENSC**  
[www.hmi.de/bensc/user-info/call-bensc\\_en.html](http://www.hmi.de/bensc/user-info/call-bensc_en.html)

**15th October 2008** **BNC-Budapest Neutron Centre**  
[www.bnc.hu/modules.php?name=News&file=article&sid=39](http://www.bnc.hu/modules.php?name=News&file=article&sid=39)

**6th October 2008** **FRJ-2 Fz-Julich**  
[www.jcns.info/jcns\\_proposals/](http://www.jcns.info/jcns_proposals/)

**25th July 2008** **FRM-II**  
<https://user.frm2.tum.de/index.php?newlang=english>

**At anytime during 2008** **GeNF-Geesthacht Neutron Facility**  
[www.gkss.de/index\\_e\\_js.html](http://www.gkss.de/index_e_js.html)

**16th September 2008 / 10th March 2009** **ILL**  
[www.ill.eu/users/experimental-programme/](http://www.ill.eu/users/experimental-programme/)

**16th April 2008** **ISIS**  
[www.isis.rl.ac.uk/applying/index.htm](http://www.isis.rl.ac.uk/applying/index.htm)

**1st October 2008** **LLB-Laboratoire Léon Brillouin**  
[www-llb.cea.fr/](http://www-llb.cea.fr/)

**15th September 2008** **NPL-Neutron Physics Laboratory**  
<http://neutron.ujf.cas.cz/>

**15th November 2008** **SINQ-Swiss Spallation Neutron**  
[http://sinq.web.psi.ch/sinq/sinq\\_call.html](http://sinq.web.psi.ch/sinq/sinq_call.html)

**September-December 2008** **SμS-Swiss Muon Source**  
<http://lmu.web.psi.ch/facilities/call2008.html>



# Synchrotron Radiation Sources

[www.lightsources.org/cms/?pid=1000336#byfacility](http://www.lightsources.org/cms/?pid=1000336#byfacility)

<b>1st November 2008</b>	<b>AS-Australian Synchrotron</b> <a href="http://www.synchrotron.org.au/content.asp?Document_ID=5305">www.synchrotron.org.au/content.asp?Document_ID=5305</a>
<b>Proposals are evaluated twice a year</b>	<b>BSRF-Beijing Synchrotron radiation Facility</b> <a href="http://www.ihep.ac.cn/bsrf/english/userinfo/beamtime.htm">www.ihep.ac.cn/bsrf/english/userinfo/beamtime.htm</a>
<b>30th September 2008</b>	<b>CFN-Center for Functional Nanomaterials</b> <a href="http://www.bnl.gov/cfn/user/proposal.asp">www.bnl.gov/cfn/user/proposal.asp</a>
<b>31st October 2008</b>	<b>CHESS-Cornell High Energy Synchrotron Source</b> <a href="http://www.chess.cornell.edu/prposals/index.htm">www.chess.cornell.edu/prposals/index.htm</a>
<b>30th September 2008</b>	<b>CLS-Canadian Light Source</b> <a href="http://www.lightsource.ca/uso/call_proposals.php">www.lightsource.ca/uso/call_proposals.php</a>
<b>31st August 2008</b>	<b>ELETTRA</b> <a href="https://vuo.elettra.trieste.it/pls/vuo/guest.startup">https://vuo.elettra.trieste.it/pls/vuo/guest.startup</a>
<b>1st December 2008</b>	<b>FELIX-Free Electron Laser for Infrared experiments</b> <a href="http://www.rijnh.nl/research/guthz/felix_felice/">www.rijnh.nl/research/guthz/felix_felice/</a>
<b>1st September 2008</b>	<b>HASYLAB-Hamburger Synchrotronstrahlungslabor at DESY</b> <a href="http://hasylab.desy.de/user_info/write_a_proposal/2_deadlines/index_eng.html">http://hasylab.desy.de/user_info/write_a_proposal/2_deadlines/index_eng.html</a>
<b>30th September 2008</b>	<b>NSRRC</b> <a href="http://portal.nsrcc.org.tw/news/news.php">http://portal.nsrcc.org.tw/news/news.php</a>
<b>15th September / 15th October 2008</b>	<b>SLS-Swiss Light Source</b> <a href="http://sls.web.psi.ch/view.php/users/experiments/proposals/opencalls/index.html">http://sls.web.psi.ch/view.php/users/experiments/proposals/opencalls/index.html</a>
<b>15th September 2008</b>	<b>SOLEIL</b> <a href="http://www.synchrotron-soleil.fr/portal/page/portal/Accueil">www.synchrotron-soleil.fr/portal/page/portal/Accueil</a>
<b>1st August 2008</b>	<b>SRC-Synchrotron Radiation Center</b> <a href="http://www.src.wisc.edu/users/Forms/proposals.htm">www.src.wisc.edu/users/Forms/proposals.htm</a>
<b>1st November / 1st December 2008</b>	<b>SSRL-Stanford Synchrotron Radiation Laboratory</b> <a href="http://www-ssrl.slac.stanford.edu/users/user_admin/deadlines.html">www-ssrl.slac.stanford.edu/users/user_admin/deadlines.html</a>

# Calendar

- August 17-21, 2008** Philadelphia, PA (USA)  
**236th American Chemical Society National Meeting & Exposition**  
[http://portal.acs.org:80/portal/acs/corg/content?\\_nfpb=true&\\_pageLabel=PP\\_TRANSITIO\\_NMAIN&node\\_id=859&use\\_sec=false&sec\\_url\\_var=region1](http://portal.acs.org:80/portal/acs/corg/content?_nfpb=true&_pageLabel=PP_TRANSITIO_NMAIN&node_id=859&use_sec=false&sec_url_var=region1)
- September 1-5, 2008** Tokai (Japan)  
**7th International Workshop on Polarized Neutrons in Condensed Matter Investigations** - <http://nsrc.tokai-sc.jaea.go.jp/pncmi2008/>
- September 1-12, 2008** Jülich (Germany)  
**12th JCNS Laboratory Course-Neutron Scattering**  
[www.fz-juelich.de/iff/wns\\_lab\\_now](http://www.fz-juelich.de/iff/wns_lab_now)
- September 7-11, 2008** Trieste (Italy)  
**LEEM-PEEM 6 Workshop** - [www.elettra.trieste.it/leempeem6/](http://www.elettra.trieste.it/leempeem6/)
- September 11-12, 2008** Warrington, Cheshire (UK)  
**UK Synchrotron Radiation User Meeting 2008**  
Daresbury Laboratory - [www.srs.ac.uk/srum08/](http://www.srs.ac.uk/srum08/)
- September 15-17, 2008** München, Garching (Germany)  
**8th German Neutron Scattering Conference 2008**  
Technische Universität  
[http://neutron.neutron-eu.net/n\\_news/n\\_calendar\\_of\\_events/n-events-2008](http://neutron.neutron-eu.net/n_news/n_calendar_of_events/n-events-2008)
- September 15-19, 2008** Pasadena, CA (USA)  
**33rd IRMMW**  
16th THz Electronics Conference - [www.irmmw-thz2008.org/](http://www.irmmw-thz2008.org/)
- September 15-19, 2008** Warsaw (Poland)  
**E-MRS Fall Meeting 2008** - <http://e-mrs.org/meetings/fall2008/>
- September 15-19, 2008** Linz (Austria)  
**NOBUGS 2008 Conference** - [www.nbi.ansto.gov.au/](http://www.nbi.ansto.gov.au/)
- September 19-22, 2008** Warsaw (Poland)  
**XTOP 2008**  
9<sup>th</sup> Biennial Conference on High Resolution X Ray Diffraction and Imaging  
[www.hlphys.jku.at/xtop2008/xtop2008.html](http://www.hlphys.jku.at/xtop2008/xtop2008.html)



- September 26-27, 2008** Stoughton, WI (USA)  
**EPDIC-11**  
European Powder Diffraction Conference - [www.epdic-11.eu/](http://www.epdic-11.eu/)
- October 7-10, 2008** Hamburg (Germany)  
**SRC Users' Meeting** - [www.lightsources.org/cms/?pid=1000068](http://www.lightsources.org/cms/?pid=1000068)
- October 9-10, 2008** Karlsruhe (Germany)  
**Interaction of Free-Electron-Laser Radiation with Matter: Recent Experimental Achievements, Challenges for Theory-Workshop**  
<https://indico.desy.de/conferenceDisplay.py?confId=798>
- October 13-14, 2008** Berkeley, CA (USA)  
**7th ANKA Users Meeting**  
[http://ankaweb.fzk.de/conferences/users\\_meeting\\_2008/first\\_page.html](http://ankaweb.fzk.de/conferences/users_meeting_2008/first_page.html)
- October 15-18, 2008** Stanford, CA (USA)  
**ALS Users' Meeting** - [www.lightsources.org/cms/?pid=1000068](http://www.lightsources.org/cms/?pid=1000068)
- October 19-23, 2008** Escandille, Autrans, near Grenoble (France)  
**2008 SSRL/LCLS Users' Meeting & Workshops**  
[www-conf.slac.stanford.edu/ssrl-lcls/2007/2008.htm](http://www-conf.slac.stanford.edu/ssrl-lcls/2007/2008.htm)
- October 19-25, 2008** Dresden (Germany)  
**Biological Physics at Large Facilities-From Molecule to Cell**  
[www.ill.eu/news-events/workshops-events/biological-physics-at-large-facilities/home/](http://www.ill.eu/news-events/workshops-events/biological-physics-at-large-facilities/home/)
- October 19-26, 2008** Hamburg (Germany)  
**2008 IEEE Nuclear Science Symposium and Medical Imaging Conference**  
[www.nss-mic.org/2008/NSSMain.asp](http://www.nss-mic.org/2008/NSSMain.asp)
- November 3-5, 2008** Ansto (Australia)  
**EMBO Practical Course on Solution Scattering from Biological Macromolecules EMBL** - [www.embl-hamburg.de/workshops/2008/embo](http://www.embl-hamburg.de/workshops/2008/embo)

# Facilities

## Neutron Scattering

WWW SERVERS IN THE WORLD  
<http://idb.neutron-eu.net/facilities.php>

### BNC Budapest Research reactor

Budapest Research Centre, Hungary  
**Type:** Swimming pool reactor, 10MW  
**Email:** [tozser@sunserv.kfki.hu](mailto:tozser@sunserv.kfki.hu)  
**http:** [//www.bnc.hu/](http://www.bnc.hu/)

### BENSIC Berlin Neutron Scattering Center

Hahn-Meitner-Institut, Glienicke Strasse 100 - D-14109 Berlin, Germany  
**Phone:** +49/30/8062-2778  
**Fax:** +49/30/8062-2523  
**E-mail:** [bensic@hmi.de](mailto:bensic@hmi.de)  
**http:** [//www.hmi.de/bensic/index\\_en.html](http://www.hmi.de/bensic/index_en.html)

### CNF

Canadian Neutron Beam Centre  
National Research Council of Canada  
Building 459, Station 18 - Chalk River Laboratories  
Chalk River, Ontario, CANADA K0J 1J0  
**Phone:** 1- (888) 243-2634 (toll free) / 1- (613) 584-8811 ext. 3973  
**Fax:** 1- (613) 584-4040  
**http:** [//cnf-ccn.gc.ca/home.html](http://cnf-ccn.gc.ca/home.html)

### FLNP - Frank Laboratory of Neutron Physics

Gpulsed reactor, mean 2 MW, pulse 1500 MW  
Joint Institute for Nuclear Research  
Dubna, Russia  
**E-mail:** [post@jinr.ru](mailto:post@jinr.ru)  
**http:** [//www.jinr.ru/](http://www.jinr.ru/)

### FRG-1 Geesthacht (D)

**Type:** Swimming Pool Cold Neutron Source  
**Flux:** 8.7 x 10<sup>13</sup> n/cm<sup>2</sup>/s  
**Address for application forms and informations:**  
Reinhard Kampmann, Institute for Materials Science  
Div. Wfn-Neutrons scattering, GKSS  
Research Centre, 21502 Geesthacht, Germany  
**Phone:** +49 (0)4152 87 1316/2503  
**Fax:** +49 (0)4152 87 1338  
**E-mail:** [reinhard.kampmann@gkss.de](mailto:reinhard.kampmann@gkss.de)  
**http:** [//www.gkss.de](http://www.gkss.de)

### FRJ-2

Forschungszentrum Jülich GmbH  
**Type:** DIDO (heavy water), 23 MW  
Research Centre Jülich, D-52425, Jülich, Germany  
**E-mail:** [info@fz-juelich.de](mailto:info@fz-juelich.de)  
**http:** [//www.fz-juelich.de/iff/wns/](http://www.fz-juelich.de/iff/wns/)

### FRM, FRM-2 (D)

Technische Universität München  
**Type:** Compact 20 MW reactor.  
**Flux:** 8 x 10<sup>14</sup> n/cm<sup>2</sup>/s  
**Address for information:** Prof. Winfried Petry  
FRM-II Lichtenbergstrasse 1-85747 Garching  
**Phone:** 089 289 14701  
**Fax:** 089 289 14666  
**E-mail:** [wpetry@frm2.tum.de](mailto:wpetry@frm2.tum.de)  
**http:** [//www.frm2.tum.de/en/index.html](http://www.frm2.tum.de/en/index.html)

### HIFIR

ORNL, Oak Ridge, USA  
**Phone:** (865)574-5231  
**Fax:** (865)576-7747  
**E-mail:** [ns\\_user@ornl.gov](mailto:ns_user@ornl.gov)  
**http:** [//neutrons.ornl.gov/](http://neutrons.ornl.gov/)

### HIFAR

ANSTO, New Illawarra Road, Lucas Heights NSW, Australia  
**Phone:** 61 2 9717 3111  
**E-mail:** [enquiries@ansto.gov.au](mailto:enquiries@ansto.gov.au)  
**http:** [//www.ansto.gov.au/information\\_about/our\\_facilities.html](http://www.ansto.gov.au/information_about/our_facilities.html)

### ILL Grenoble (F)

**Type:** 58MW High Flux Reactor  
**Flux:** 1.5 x 10<sup>15</sup> n/cm<sup>2</sup>/s  
**Scientific Coordinator:** Dr. G. Cicognani, ILL, BP 156,  
38042 Grenoble Cedex 9, France  
**Phone:** +33 4 7620 7179  
**Fax:** +33 4 76483906  
**E-mail:** [cico@ill.fr](mailto:cico@ill.fr) and [sco@ill.fr](mailto:sco@ill.fr)  
**http:** [//www.ill.fr](http://www.ill.fr)

### IPNS Intense Pulsed Neutron at Argonne

**for proposal submission by e-mail**  
**send to [cpeters@anl.gov](mailto:cpeters@anl.gov) or mail/fax to:**  
IPNS Scientific Secretary, Building 360  
Argonne National Laboratory, 9700 South Cass Avenue, Argonne,  
IL 60439-4814, USA  
**Phone:** 630/252-7820  
**Fax:** 630/252-7722  
**http:** [//www.pns.anl.gov/](http://www.pns.anl.gov/)

### ISIS Didcot

**Type:** Pulsed Spallation Source.  
**Flux:** 2.5 x 10<sup>16</sup> n fast/s  
**Address for application forms:**  
ISIS Users Liaison Office, Building R3,  
Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, UK  
**Phone:** +44 (0) 1235 445592  
**Fax:** +44 (0) 1235 445103  
**E-mail:** [uls@isis.rl.ac.uk](mailto:uls@isis.rl.ac.uk)  
**http:** [//www.isis.rl.ac.uk](http://www.isis.rl.ac.uk)





### JRR-3M

Tokai-mura, Naka-gun, Ibaraki-ken 319-11, Japan  
Jun-ichi Suzuki, JAERI-Japan Atomic Energy Research Institute  
Yuji Ito (ISSP, Univ. of Tokyo)  
**Fax:** +81 292 82 59227  
**Telex:** JAERIJ24596  
**E-mail:** www-admin@www.jaea.go.jp  
**http://**ciscpyon.tokai-sc.jaea.go.jp/english/index.cgi

### JEEP-II Reactor Kjeller

**Type:** D2O moderated 3.5% enriched UO2 fuel  
**Flux:** 2 x 10<sup>13</sup> n/cm<sup>2</sup>/s  
**Address for application forms:**  
Institut for Energiteknikk  
K.H. Bendiksen, Managing Director, Box 40, 2007 Kjeller, Norway  
**Phone:** +47 63 806000, 806275  
**Fax:** +47 63 816356  
**E-mail:** kjell.bendiksen@ife.no  
**http://**www.ife.no

### KENS

Institute of Materials Structure Science  
High Energy Accelerator research Organisation  
1-1 Oho, Tsukuba-shi, Ibaraki-ken, 305-0801, JAPAN  
**E-mail:** kens-pac@nml.kek.jp  
**http://**neutron-www.kek.jp/index\_e.html

### KUR-Kyoto University Research Reactor Institute

Kumatori-cho Sennan-gun, Osaka 590-0494, Japan  
**Phone:** +81-72-451-2300  
**Fax:** +81-72-451-2600  
**http://**www.rii.kyoto-u.ac.jp/en/

### LANSCE

Los Alamos Neutron Science Center  
TA-53, Building 1, MS H831, Los Alamos National Lab, Los Alamos, USA  
**Phone:** +1 505-665-8122  
**E-mail:** tichavez@lanl.gov  
**http://**www.lansce.lanl.gov/index.html

### LLB Orphée Saclay (F)

**Type:** Reactor. Flux: 3.0 x 10<sup>14</sup> n/cm<sup>2</sup>/s  
Laboratoire Léon Brillouin (CEA-CNRS)  
**E-mail:** experience@llb.saclay.cea.fr  
**http://**www-llb.cea.fr/index\_e.html

### NFL – Studsvick Neutron Research Laboratory

Uppsala University-Studsvik Nuclear AB, Stockholm, Sweden  
**Type:** swimming pool type reactor, 50 MW, with additional reactor 1 MW  
**http://**idb.neutron-eu.net/facilities.php

### NCNR-NIST Center for Neutron Research

National Institute of Standards and Technology  
100 Bureau Drive, MS 8560 - Gaithersburg, MD 20899-8560, USA  
Patrick Gallagher, Director  
**Phone:** (301) 975-6210  
**Fax:** (301) 869-4770  
**E-mail:** pgallagher@nist.gov  
**http://**rrdjazz.nist.gov/

### NPL – NRI

**Type:** 10 MW research reactor.  
**Address for informations:**  
Zdenek Kriz, Scientific Secretary, Nuclear Research Institute Rez plc, 250 68  
Rez-Czech Republic  
**Phone:** +420 2 20941177 / 66173428  
**Fax:** +420 2 20941155  
**E-mail:** krz@ujv.cz and brv@nri.cz  
**http://**www.nri.cz

### NRU Chalk River Laboratories

The peak thermal flux 3x10<sup>14</sup> cm<sup>-2</sup> sec<sup>-1</sup>  
Neutron Program for Materials Research  
National Research Council Canada  
Building 459, Station 18, Chalk River Laboratories, Chalk River  
Ontario-Canada K0J 1J0  
**Phone:** 1-(888) 243-2634 (toll free)  
**Phone:** 1-(613) 584-8811 ext. 3973  
**Fax:** 1- (613) 584-4040  
**http://**neutron.nrc-cnrc.gc.ca/home.html

### RID Reactor Institute Delft (NL)

**Type:** 2MW light water swimming pool.  
**Flux:** 1.5 x 10<sup>13</sup> n/cm<sup>2</sup>/s  
**Address for application forms:**  
Dr. M. Blaauw, Head of Facilities and Services Dept.  
Reactor Institute Delft, Faculty of Applied Sciences  
Delft University of Technology, Mekelweg 15  
2629 JB Delft, The Netherlands  
**Phone:** +31-15-2783528  
**Fax:** +31-15-2788303  
**E-mail:** m.blaauw@tudelft.nl  
**http://**www.rid.tudelft.nl

### SINQ Villigen (CH)

**Type:** Steady spallation source  
**Flux:** 2.0 x 10<sup>14</sup> n/cm<sup>2</sup>/s  
**Contact address:** PSI-Paul Scherrer Institut  
User Office, CH-5232 Villigen PSI, Switzerland  
**Phone:** +41 56 310 4666  
**Fax:** +41 56 310 3294  
**E-mail:** sinq@psi.ch  
**http://**sinq.web.psi.ch

### SNS – Spallation Neutron Source

ORNL, Oak Ridge, USA  
**Address for information:**  
Allen E. Ekkebus  
Spallation Neutron Source, Oak Ridge National Laboratory  
One Bethel Valley Road, Bldg 8600 - P.O. Box 2008, MS 6460  
Oak Ridge, TN 37831-6460  
**Phone:** (865) 241-5644  
**Fax:** (865) 241-5177  
**E-mail:** ekkebusae@ornl.gov  
**http://**www.sns.gov/

# Synchrotron Radiation Sources

WWW SERVERS IN THE WORLD  
www.lightsources.org/cms/?pid=1000098

## ALBA-Synchrotron Light Facility

CELLS-ALBA  
Edifici Ciències. C-3 central. Campus UAB  
Campus Universitari de Bellaterra. Universitat Autònoma de Barcelona  
08193 Bellaterra, Barcelona Spain  
**Phone:** +34 93 592 43 00  
**Fax:** +34 93 592 43 01  
**http://www.cells.es/**

## ALS Advanced Light Source

Berkeley Lab, 1 Cyclotron Rd, MS6R2100, Berkeley, CA 94720  
**Phone:** +1 510.486.7745  
**Fax:** +1 510.486.4773  
**E-mail:** alsuser@lbl.gov  
**http://www-als.lbl.gov/als/**

## ANKA

Forschungszentrum Karlsruhe Institut für Synchrotronstrahlung  
Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen,  
Germany  
**Phone:** +49 (0)7247 / 82-6071  
**Fax:** +49-(0)7247 / 82-6172  
**E-mail:** info@fzk.de  
**http://ankaweb.fzk.de/**

## APS Advanced Photon Source

Argonne Nat. Lab. 9700 S. Cass Avenue, Argonne, IL 60439, USA  
**Phone:** (630) 252-2000  
**Fax:** +1 708 252 3222  
**E-mail:** fenner@aps.anl.gov  
**http://www.aps.anl.gov/**

## AS Australian Synchrotron

Level 17, 80 Collins St, Melbourne VIC 3000, Australia  
**Phone:** +61 3 9655 3315  
**Fax:** +61 3 9655 8666  
**E-mail:** contact.us@synchrotron.vic.gov.au  
**http://www.synchrotron.vic.gov.au/content.asp?Document\_ID=1**

## BESSY Berliner Elektronenspeicherring Gesellschaft für Synchrotronstrahlung

BESSY GmbH, Albert-Einstein-Str.15, 12489 Berlin, Germany  
**Phone:** +49 (0)30 6392-2999  
**Fax:** +49 (0)30 6392-2990  
**E-mail:** info@bessy.de  
**http://www.bessy.de/**

## BSRF Beijing Synchrotron Radiation Facility

BEPC National Laboratory, Institute of High Energy Physics, Chinese  
Academy of Sciences  
P.O.Box 918, Beijing 100039, P. R. China  
**Phone:** +86-10-68235125  
**Fax:** +86-10-68222013  
**E-mail:** houbz@mail.ihep.ac.cn  
**http://www.ihep.ac.cn/bsrf/english/main/main.htm**

## CAMD Center Advanced Microstructures & Devices

CAMD/LSU 6980 Jefferson Hwy., Baton Rouge, LA 70806, USA  
**Phone:** +1 (225) 578-8887  
**Fax:** +1 (225) 578-6954  
**E-mail:** leeann@lsu.edu  
**http://www.camd.lsu.edu/**

## CANDLE Center for the Advancement of Natural Discoveries using Light Emission

Acharyan 31, 375040, Yerevan, Armenia  
**Phone/fax:** +374-1-629806  
**E-mail:** baghiryan@asls.candle.am  
**http://www.candle.am/index.html**

## CESLAB – Central European Synchrotron Laboratory

**Contact:** Assoc. Prof. RNDr. Stanislav Kozubek, DrSc.  
Director of the Institute of Biophysics AS CR, v.v.i  
Kralovopolska 135, 612 65 Brno, Czech Republic  
**Phone:** +420-541517500  
**E-mail:** kozubek@ibp.cz  
**http://www.synchrotron.cz/synchrotron/Central\_European\_Synchrotron\_Laboratory\_\_\_\_\_EN.html**

## CFN – Center for Functional Nanomaterials

User Administration Office  
Brookhaven National Laboratory  
P.O. Box 5000, Bldg. 555  
Upton, NY 11973-5000, USA  
**Phone:** +1 (631) 344-6266  
**Fax:** +1 (631) 344-3093  
**E-mail:** cfnuser@bnl.gov  
**http://www.bnl.gov/cfn/**

## CHESS Cornell High Energy Synchrotron Source

Cornell High Energy Synchrotron Source  
200L Wilson Lab, Rt. 366 & Pine Tree Road, Ithaca, NY 14853, USA  
**Phone:** +1 (607) 255-7163 ?/ +1 (607) 255-9001  
**http://www.chess.cornell.edu/**

## CLIO – Centre Laser Infrarouge d'Orsay

CLIO/LCP  
Bat. 201-P2 - Campus Universitaire, 91405 ORSAY Cedex, France  
**http://www.lcp.u-psud.fr/clio/clio\_eng/clio\_eng.htm**



### CLS Canadian Light Source

Canadian Light Source Inc., University of Saskatchewan  
101, Perimeter Road Saskatoon, SK., Canada. S7N 0X4

**Phone:** (306) 657-3500

**Fax:** (306) 657-3535

**E-mail:** [clsuo@lightsource.ca](mailto:clsuo@lightsource.ca)

**http://www.lightsource.ca/**

### CNM – Center for Nanoscale Materials

Argonne National Laboratory  
9700 S. Cass Avenue. Bldg. 440  
Argonne, IL 60439, USA

**Phone:** (630) 252-2000

**http://nano.anl.gov/facilities/index.html**

### CTST-UCSB Center for Terahertz Science and Technology

University of California, Santa Barbara (UCSB), USA

**http://sbfel3.ucsb.edu/**

### DAFNE Light

INFN – LNF

Via Enrico Fermi, 40, I-00044 Frascati (Rome), Italy

**Fax:** +39 6 94032597

**http://www.lnf.infn.it/esperimenti/sr\_dafne\_light/**

### DELSY Dubna Electron Synchrotron

JINR Joliot-Curie 6, 141980 Dubna, Moscow region, Russia

**Phone:** + 7 09621 65 059

**Fax:** + 7 09621 65 891

**E-mail:** [post@jinr.ru](mailto:post@jinr.ru)

**http://www.jinr.ru/delsy/**

### DELTA Dortmund Electron Test Accelerator-FELICITA I (FEL)

Institut für Beschleunigerphysik und Synchrotronstrahlung  
Universität Dortmund

Maria-Goeppert-Mayer-Str. 2, 44221 Dortmund, Germany

**Fax:** +49-(0)231-755-5383

**http://www.delta.uni-dortmund.de/index.php?id=2&L=1**

### DFELL Duke Free Electron Laser Laboratory

Duke Free Electron Laser Laboratory  
PO Box 90319, Duke University Durham  
North Carolina 27708-0319, USA

**Phone:** 1 (919) 660-2666

**Fax:** +1 (919) 660-2671

**E-mail:** [beamtime@fel.duke.edu](mailto:beamtime@fel.duke.edu)

**http://www.fel.duke.edu/**

### Diamond Light Source

Diamond Light Source Ltd  
Diamond House, Chilton, Didcot, OXON, OX11 0DE, UK

**Phone:** +44 (0)1235 778000

**Fax:** +44 (0)1235 778499

**E-mail:** [useroffice@diamond.ac.uk](mailto:useroffice@diamond.ac.uk)

**http://www.diamond.ac.uk/default.htm**

### ELETTRA Synchrotron Light Lab.

Sincrotrone Trieste S.C.p.A

Strada Statale 14-Km 163,5 in AREA Science Park

34012 Basovizza, Trieste, Italy

**Phone:** +39 40 37581

**Fax:** +39 (040) 938-0902

**http://www.elettra.trieste.it/**

### ELSA Electron Stretcher Accelerator

Physikalisches Institut der Universität Bonn

Beschleunigeranlage ELSA, Nußallee 12, D-53115 Bonn, Germany

**Phone:** +49-228-735926

**Fax:** +49-228-733620

**E-Mail:** [roy@physik.uni-bonn.de](mailto:roy@physik.uni-bonn.de)

**http://www-elsa.physik.uni-bonn.de/elsa-facility\_en.html**

### ESRF European Synchrotron Radiation Lab.

ESRF, 6 Rue Jules Horowitz, BP 220, 38043 Grenoble Cedex 9, France

**Phone:** +33 (0)4 7688 2000

**Fax:** +33 (0)4 7688 2020

**E-mail:** [useroff@esrf.fr](mailto:useroff@esrf.fr)

**http://www.esrf.eu/**

### FELBE Free-Electron Lasers at the ELBE radiation source at the FZR/Dresden

Bautzner Landstrasse 128, 01328 Dresden, Germany

**http://www.fzd.de/db/Cms?pNid=471**

### FELIX Free Electron Laser for Infrared eXperiments

FOM Institute for Plasma Physics 'Rijnhuizen'

Edisonbaan, 14, 3439 MN Nieuwegein, The Netherlands

P.O. Box 1207, 3430 BE Nieuwegein, The Netherlands

**Phone:** +31-30-6096999

**Fax:** +31-30-6031204

**E-mail:** [B.Redlich@rijnh.nl](mailto:B.Redlich@rijnh.nl)

**http://www.rijnh.nl/felix/**

### HASYLAB Hamburger Synchrotronstrahlungslabor-DORIS III, PETRA II / III, FLASH

DESY-HASYLAB

Notkestrasse 85, 22607 Hamburg, Germany

**Phone:** +49 40 / 8998-2304

**Fax:** +49 40 / 8998-2020

**E-mail:** [HASYPALB@DESY.de](mailto:HASYLAB@DESY.de)

**http://hasylab.desy.de/**

### HSRC Hiroshima Synchrotron Radiation Center-HiSOR

Hiroshima University

2-313 Kagamiyama, Higashi-Hiroshima, 739-8526, Japan

**Phone:** +81 82 424 6293

**Fax:** +81 82 424 6294

**http://www.hsrb.hiroshima-u.ac.jp/english/index-e.htm**

**iFEL**

Institute of Free Electron Laser, Graduate School of Engineering  
Osaka University

2-9-5 Tsuda-Yamate, Hirakata, Osaka 573-0128, Japan

**Phone:** +81-(0)72-897-6410

**http://www.fel.eng.osaka-u.ac.jp/english/index\_e.html**

**INDUS -1 / INDUS -2**

Centre for Advanced Technology Department of Atomic Energy  
Government of India

**P.O.:** CAT Indore, M.P-452 013, India

**Phone:** +91-731-248-8003

**Fax:** 91-731-248-8000

**E-mail:** rvn@cat.ernet.in

**http://www.cat.ernet.in/technology/accel/indus/index.html**

**http://www.cat.ernet.in/technology/accel/atdhome.html**

**IR FEL Research Center-FEL-SUT**

IR FEL Research Center, Research Institutes for Science and Technology

The Tokyo University of Science, Yamazaki 2641, Noda

Chiba 278-8510, Japan

**Phone:** +81 4-7121-4290

**Fax:** +81 4-7121-4298

**E-mail:** felsut@rs.noda.sut.ac.jp

**http://www.rs.noda.sut.ac.jp/~felsut/english/index.htm**

**ISA Institute for Storage Ring Facilities-ASTRID-1**

ISA, University of Aarhus, Ny Munkegade, bygn. 520

DK-8000 Aarhus C, Denmark

**Phone:** +45 8942 3778

**Fax:** +45 8612 0740

**E-mail:** fyssp@phys.au.dk

**http://www.isa.au.dk/**

**ISI-800**

Institute of Metal Physics

National Academy of Sciences of Ukraine

**Phone:** +(380) 44 424-1005

**Fax:** +(380) 44 424-2561

**E-mail:** metall@imp.kiev.ua

**Jlab-Jefferson Lab FEL**

12000 Jefferson Avenue, Newport News, Virginia 23606, USA

**Phone:** (757) 269-7767

**http://www.jlab.org/FEL**

**Kharkov Institute of Physics and Technology-Pulse Stretcher/Synchrotron Radiation**

National Science Center, KIPT, 1

Akademicheskaya St., Kharkov, 61108, Ukraine

**http://www.kipt.kharkov.ua/.indexe.html**

**KSR-Nuclear Science Research Facility-Accelerator Laboratory**

Gokasho,Uji, Kyoto 611

**Fax:** +81-774-38-3289

**http://www.wal.kuicr.kyoto-u.ac.jp/www/index-e.htmlx**

**KSRS Kurchatov Synchrotron Radiation Source****KSRS-Siberia-1 / Siberia-2**

Kurchatov Institute 1

Kurchatov Sq., Moscow 123182, Russia

**http://www.kiae.ru/**

**LCLS Linac Coherent Light Source**

Stanford Linear Accelerator Center (SLAC)

2575 Sand Hill Road, MS 18, Menlo Park, CA 94025, USA

**Phone:** +1 (650) 926-3191

**Fax:** +1 (650) 926-3600

**E-mail:** knotts@ssrl.slac.stanford.edu

**http://www-ssrl.slac.stanford.edu/lcls/**

**LNLS Laboratorio Nacional de Luz Sincrotron**

Caixa Postal 6192, CEP 13084-971, Campinas, SP, Brazil

**Phone:** +55 (0) 19 3512-1010

**Fax:** +55 (0)19 3512-1004

**E-mail:** sau@lnls.br

**http://www.lnls.br/index.asp?idioma=2&opcaoescq**

**MAX-Lab**

Box 118, University of Lund, S-22100 Lund, Sweden

**Phone:** +46-222 9872

**Fax:** +46-222 4710

**http://www.maxlab.lu.se/**

**Medical Synchrotron Radiation Facility**

National Institute of Radiological Sciences (NIRS)

4-9-1, Anagawa, Inage-ku, Chiba-shi, 263-8555, Japan

**Phone:** +81-(0)43-251-2111

**http://www.nirs.go.jp/ENG/index.html**

**MLS – Metrology Light Source**

Physikalisch-Technische Bundesanstalt

Willy-Wien-Laboratorium

Magnusstraße 9, 12489 Berlin, Germany

**Phone:** +49 30 3481 7312

**Fax:** +49 30 3481 7550

**Email:** Gerhard.Ulm@ptb.de

**http://www.ptb.de/mls/**

**NSLS National Synchrotron Light Source**

NSLS User Administration Office

Brookhaven National Laboratory, P.O. Box 5000, Bldg. 725B, Upton, NY

11973-5000, USA

**Phone:** +1 (631) 344-7976

**Fax:** +1 (631) 344-7206

**E-mail:** nslsuser@bnl.gov

**http://www.nsls.bnl.gov/**

**NSRL National Synchrotron Radiation Lab.**

University of Science and Technology China (USTC)

Hefei, Anhui 230029, PR China

**Phone:** +86-551-3601989

**Fax:** +86-551-5141078

**E-mail:** zdh@ustc.edu.cn

**http://www.nsrl.ustc.edu.cn/en/**



### **NSRRC National Synchrotron Radiation Research Center**

National Synchrotron Radiation Research Center  
101 Hsin-Ann Road, Hsinchu Science Park, Hsinchu 30076, Taiwan, R.O.C.  
**Phone:** +886-3-578-0281  
**Fax:** +886-3-578-9816  
**E-mail:** user@nsrrc.org.tw  
**http://www.nsrrc.org.tw/**

### **NSSR Nagoya University Small Synchrotron Radiation Facility**

Nagoya University  
4-9-1, Anagawa, Inage-ku, Chiba-shi, 263-8555, Japan  
**Phone:** +81-(0)43-251-2111  
**http://www.nagoya-u.ac.jp/en/**

### **PAL Pohang Accelerator Lab.**

San-31 Hyoja-dong Pohang, Kyungbuk 790-784, Korea  
**http://pal.postech.ac.kr/eng/index.html**

### **PF Photon Factory**

KEK, 1-1 Oho, Tsukuba, Ibaraki 305-0801, Japan  
**Phone:** +81 (0)-29-879-6009  
**Fax:** +81 (0)-29-864-4402  
**E-mail:** users.office2@post.kek.jp  
**http://pfwww.kek.jp/**

### **PSLS-Polish Synchrotron Light Source**

Centrum Promieniowania Synchrotronowego Sp. z o.o.  
ul. Reymonta 4, PL-30-059 Kraków  
**Phone:** +48 (12) 663 58 20  
**E-mail:** mail@synchrotron.pl  
**http://www.if.uj.edu.pl/Synchro/**

### **RitS Ritsumeikan University SR Center**

Ritsumeikan University (RitS) SR Center  
Biwako-Kusatsu Campus, Noji Higashi 1-chome, 1-1 Kusatsu  
525-8577 Shiga-ken, Japan  
**Phone:** +81 (0)77 561-2806  
**Fax:** +81 (0)77 561-2859  
**E-mail:** d11-www-adm@se.ritsumeik.ac.jp  
**http://www.ritsumeik.ac.jp/se/re/SLLS/newpage13.htm**

### **SAGA-LS-Saga Light Source**

Kyushu Synchrotron Light Research Center  
8-7 Yayoigaoka, Tosu, Saga 841-0005, Japan  
**Phone:** +81-942-83-5017  
**Fax:** +81-942-83-5196  
**http://www.saga-ls.jp/english/index.htm**

### **SESAME Synchrotron-light for Experimental Science and Applications in the Middle East**

**E-mail:** hhelal@mail.eun.edu  
**http://www.sesame.org.jo/index.aspx**

### **SLS Swiss Light Source**

Paul Scherrer Institut reception building, PSI West, CH-5232 Villigen PSI, Switzerland  
**Phone:** +41 56 310 4666  
**Fax:** +41 56 310 3294  
**E-mail:** slsuo@psi.ch  
**http://sls.web.psi.ch/view.php/about/index.html**

### **SOLEIL**

Synchrotron SOLEIL  
L'Orme des Merisiers  
Saint-Aubin-BP 48 91192 GIF-sur-YVETTE CEDEX, FRANCE  
**Phone:** +33 1 6935 9652  
**Fax:** +33 1 6935 9456  
**E-mail:** frederique.fraissard@synchrotron-soleil.fr  
**http://www.synchrotron-soleil.fr/**

### **SPL-Siam Photon Laboratory**

The Siam Photon Laboratory of the National Synchrotron Research Center  
111 University Avenue, Muang District, Nakhon Ratchasima 30000, Thailand  
**Postal Address:** PO. BOX 93, Nakhon Ratchasima 30000, Thailand  
**Phone:** +66-44-21-7040  
**Fax:** +66-44-21-7047, +66-44-21-7040 ext 211  
**http://www.nsrc.or.th/eng/**

### **SPring-8**

Japan Synchrotron Radiation Research Institute (JASRI)  
Kouto, Sayo-cho, Sayo-gun, Hyogo 679-5198, Japan  
**Phone:** +81-(0) 791-58-0961  
**Fax:** +81-(0) 791-58-0965  
**E-mail:** sp8jasri@spring8.or.jp  
**http://www.spring8.or.jp/en/**

### **SRC-Synchrotron Radiation Center**

Synchrotron Radiation Center  
3731 Schneider Dr., Stoughton, WI 53589-3097, USA  
**Phone:** +1 (608) 877-2000  
**Fax:** +1 (608) 877-2001  
**http://www.src.wisc.edu/**

### **SRS-Synchrotron Radiation Source**

CCLRC Daresbury Laboratory, Warrington, Cheshire, UK. WA4 4AD  
**Phone:** +44 (0)1925 603223  
**Fax:** +44 (0)1925 603174  
**E-mail:** srs-ulo@dl.ac.uk  
**http://www.srs.ac.uk/srs/**

### **SSLS Singapore Synchrotron Light Source –Helios II**

National University of Singapore (NUS)  
Singapore Synchrotron Light Source, National University of Singapore  
5 Research Link, Singapore 117603, Singapore  
**Phone:** (65) 6874-6568  
**Fax:** (65) 6773-6734  
**http://ssls.nus.edu.sg/index.html**



**SSRC Siberian Synchrotron Research Centre – VEPP3/VEPP4**

Lavrentyev av. 11, Budker INP, Novosibirsk 630090, Russia

**Phone:** +7(3832)39-44-98**Fax:** +7(3832)34-21-63**E-mail:** G.N.Kulipanov@inp.nsk.su**http://ssrc.inp.nsk.su/english/load.pl?right=general.html****SSRF-Shanghai Synchrotron Radiation Facility****http://ssrf.sinap.ac.cn/english/****SSRL Stanford Synchrotron Radiation Lab.**

Stanford Linear Accelerator Center, 2575 Sand Hill Road, Menlo Park, CA 94025, USA

**Phone:** +1 650-926-3191**Fax:** +1 650-926-3600**E-mail:** knotts@ssrl.slac.stanford.edu**http://www-ssrl.slac.stanford.edu/users/user\_admin/ura\_staff\_new.html****Stanford Picosecond FEL Center****http://www.stanford.edu/group/FEL/****SuperSOR-SuperSOR Synchrotron Radiation Facility**

Synchrotron Radiation Laboratory

Institute for Solid State Physics,

The University of Tokyo

5-1-5 Kashiwa-no-ha, Kashiwa, Chiba 277-8581, Japan

**Phone:** +81 (0471) 36-3405**Fax:** +81(0471) 34-6041**E-mail:** kakizaki@issp.u-tokyo.ac.jp**http://www.issp.u-tokyo.ac.jp/labs/sor/project/MENU.html****SURF-II / SURF-III Synchrotron Ultraviolet Radiation Facility**

NIST, 100 Bureau Drive, Stop 3460, Gaithersburg

MD 20899-3460, USA

**Phone:** +1 (301) 975-4200**http://physics.nist.gov/MajResFac/SURF/SURF/index.html****TNK-F.V. Lukin Institute**

State Research Center of Russian Federation

103460, Moscow, Zelenograd

**Phone:** +7(095) 531-1306 / +7(095) 531-1603**Fax:** +7(095) 531-4656**E-mail:** admin@niifp.ru**http://www.niifp.ru/index\_e.html****TSRF Tohoku Synchrotron Radiation Facility-Laboratory of Nuclear Science**

Tohoku University

**Phone:** +81 (022)-743-3400**Fax:** +81 (022)-743-3401**E-mail:** koho@LNS.tohoku.ac.jp**http://www.lns.tohoku.ac.jp/index.php****UVSOR Ultraviolet Synchrotron Orbital Radiation Facility**

UVSOR Facility, Institute for Molecular Science, Myodaiji

Okazaki 444-8585, Japan

**http://www.uvsor.ims.ac.jp/defaultE.html****VU FEL W. M. Keck Vanderbilt Free-electron Laser Center**

410 24th Avenue, Nashville, TN 37212, Box 1816, Stn B

Nashville, TN 37235, USA

**http://www.vanderbilt.edu/fel/****INFORMATION**

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