

SHUG (SNS HFIR User Group), <http://neutrons.ornl.gov/users/shug/>
SHUG executive committee minutes.

Teleconference held April 5, 2011.

Attendees:

Executive Committee: Cora Lind, Matthew Stone, Greg Beaucage, Eugenia Kharlampieva, Malcolm Guthrie and Mike Crawford.

Guests: Ken Herwig, Mike Simonson, Al Ekkebus

Minutes submitted for review April 7, 2011 by M. B. Stone.

ACTION ITEMS:

- Please note next telecon date: May 3, 2011 at 1 PM

ATTACHMENTS and WEBSITES of interest from the teleconference:

Proposed Quarterly Neutron News electronic publication.

Two neutron scattering opportunities of interest

1. Update for HFIR and SNS (Ken and Mike)

The liquid mercury target vessel at the SNS had a designed failure occur on the morning of Sunday April 3. The two lifetime limits of the target are the radiation damage to the outer container, and cavitation damage from the mercury inside the target. Part of the original plan for operation of the SNS at high beam power was to change up to 4 of these targets per year. In order to learn about the lifetimes of targets, the decision was made to run this target to its designed failure. The replacement has already begun. This will be an approximate two week interruption of the user program. These two weeks will be made up by adding operating days during the current summer outage. Neutron production will likely begin on April 17th, with user operation to start April 19th or 20th. Messages have been sent to the potentially impacted users. Another message will be sent to a broader list of individuals. This was a planned event, the facility just did not know when it would occur.

The target vessel which failed was first installed in the late summer of 2010. This target vessel accumulated more operating hours at a higher power level. About 22 tons of mercury circulates through the target.

HFIR is in the midst of its long outage. The general purpose SANS detector is being replaced with a multi-tube detector which should give an improved count-rate of a factor of 40. This may allow additional experiments to be performed. This is a second generation of the SNS SANS detector.

Instruments are still being commissioned at the SNS, and progress is continually being made.

The J-PARC MLF neutron scattering facility was damaged due to the recent earthquake in Japan. The SNS will be working with our colleagues in Japan to determine which high priority experiments can be done at the SNS facility that were scheduled to be run at J-PARC. These choices will be made in consultation with J-PARC staff, NSSD management, and the beamtime allocation committee.

There has been a new hire for the Center for Structural Molecular Biology, Paul Longan will begin as group leader on April 11.

The guest house is scheduled to be completed in summer 2011.

2. Quarterly Neutron News handout (AI, see e-mail attachment from AI this week)

Many organizations have periodic messages to their user communities which include science highlights, notes from the director, and information for people's calendars. AI Ekkebus has circulated a potential format of a Quarterly Neutron News electronic publication. Current items are a "Directors Note", "Facility Summary", "Science Highlights" and news.

A copy of this proposed format is attached to these minutes.

It was suggested to include small pictures of the new staff members who will be interacting with the users, It would also be nice to include a series of important dates or conferences. Going beyond four pages would be considered too long. Three pages is a good balance. A title and a date should be included at the top of the banner. A bimonthly or quarterly release would be reasonable. An advertisement for submission of highlights should be added, and the next proposal submission deadline should be emphasized.

3. National User Facility Organization meeting in Washington, D.C. (AI, Cora)

NSSD is sending Ian Anderson, Cora Lind and Despina Louca to the NUFO meeting in Washington D.C. on Thursday April 7, 2011. This was initiated by representatives Birggert and Holt, and is for the benefit of members of congress and their staff. There will be posters representing 37 different facilities including HFIR and SNS. See the NUFO website <http://nufo.org> for additional information.

4. Regional conferences? (All)

Last month it was generally felt that sending neutron scattering information from the division to regional meetings would be a good idea to recruit new users.

The North American Solid State Conference in Hamilton, Ontario, Canada in early June is one example of a potential meeting to send materials with SHUG members for presentation of information.

5. Other business?

* Next telecon date
Tuesday MAY 3, 2011 at 1 PM



Director's Note

Scientific output from HFIR and SNS included more than 200 journal articles. SNS hosted 422 and HFIR hosted 375 unique on-site users and there was also significant usage of remote access to instruments and data analysis by off-site users. Projects funded by industry increased 34 in 2010. HFIR now has 10 operational instruments, all available to users. SNS has 13 operational instruments, 7 of which are in the user program with the other 6 in commissioning. The new complex of 13 laboratories on the second floor of the SNS Central Laboratory and Office Building opened to users in the fall.

I would like the staff and users for their attention to safety during the last year.

Jan Anderson

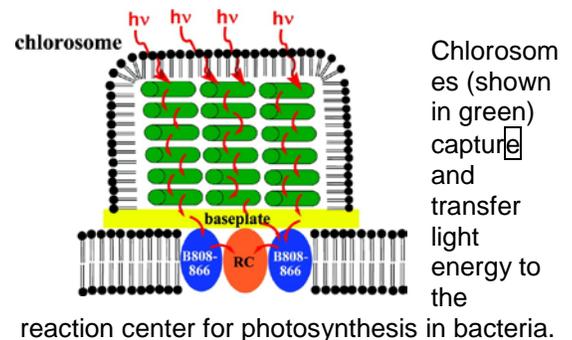
Facility Summary

At HFIR, Cycle 432 ended December 17, 2010, and Cycle 433 began January 10, 2011. The HFIR long-term schedule is [available](#). At SNS, the current cycle of neutron production ended December 20, 2010, and will resume February 14, 2011. The detailed SNS schedule is [available](#). Recent availability is approaching 95%.

Science Highlights

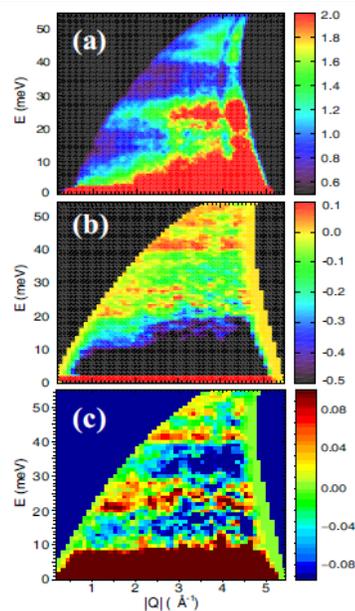
Effects of temperature and ionic strength on chlorosome of green photosynthetic bacteria

The Bio-SANS at HFIR was used to examine chlorosome structure of a green photosynthetic bacteria under a range of thermal and ionic conditions. Results showed the structure to be stable under all tested conditions. *C. aurantiacus* chlorosomes remained intact at temperatures up to 70°C. This is in contrast to free chlorophylls, which have been found to break down at temperatures above 42 °C. The results also showed chlorosomes to be stable in a pH range of 5.5 to 11. The size, shape and organization of light-harvesting complexes such as chlorosomes are critical in electron transfer to semiconductor electrodes in solar devices. Understanding how chlorosomes function in nature could help in creating robust bio-inspired solar cells. **Details**



SEQUOIA measures magnetic excitation spectrum in TiOBr

Neutron scattering detected and measured the magnetic excitation spectrum of TiOBr, an oxyhalogen with a rare phase transition. Results from the time-of-flight chopper spectrometer SEQUOIA at SNS revealed two branches of magnetic excitations in the material. This is the first direct measure of the singlet-triplet energy gap. The bandwidth of the excitations is relatively narrow compared with the size of the singlet-triplet energy gap, suggesting that the excitations are well-localized. The interactions between excited triplets appear to be small. The results will help to guide and inform future studies of these novel magnetic systems. Details



Maps of inelastic neutron scattering intensity, $S(Q,E)$, for TiOBr at $T = 8\text{K}$. (a) $S(Q,E)$ after empty can background subtraction to eliminate scattering from sample environment. (b) $S(Q,E)$ after high temperature (80 K) background subtraction to isolate magnetic scattering. (c) $S(Q,E)$ after high temperature background subtraction weighted by an appropriate Bose correction.

Stimuli-responsive behavior in polyelectrolyte dendrimers revealed by neutron scattering

Researchers used neutron scattering at HFIR and SNS to understand the relationship between molecular charge and properties when polyelectrolyte dendrimers are in aqueous solution. This charge-stimulated response may be used in biomedical and sustainable energy applications. The BASIS dynamics study at SNS shows that when the molecular charge increases, a significant enhancement occurs in the local dynamics. The SANS structural study at HFIR shows that a gradual increase occurs in the molecular size with a continuous redistribution of the intra-molecular density. The findings provide the microscopic picture needed to develop polyelectrolyte dendrimers for specific targeted functions. Details

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Neutron Science in the News

<http://neutrons.ornl.gov/media/news/current-news.shtml>

Meetings and Events

<http://neutrons.ornl.gov/calendar/>

HFIR and SNS Contacts

User Office: 865.574.4600

Email: neutronusers@ornl.gov
<http://neutrons.ornl.gov/users/contacts.shtml>

Join our mailing list:

http://erie.ornl.gov/sns_users/AddedUsers.cfm

Collaborative Research

<http://neutrons.ornl.gov/crv/>

Oak Ridge National Laboratory



New or Expanded Capabilities

 **First user of SNS labs.** Mike Crawford, a chemist at DuPont who's a regular at SNS and HFIR, was the first outside user to take advantage of the new SNS second-floor laboratory suite. [See the highlight.](#)

Instruments, People and Users

 Three ORNL neutron scattering users were recently named Fellows of the American Physical Society: Robert McQueeney, Iowa State University (development and use of neutron scattering techniques to advance the understanding of strongly correlated electron systems), Dave Christen, ORNL (sustained discovery and leadership in understanding of superconductive materials, especially their current conduction and vortex state properties), and Xun-Li Wang, of structure, phase transformations, and mechanical behavior in materials and engineering systems and leadership in the design and construction of a versatile engineering diffractometer at the Spallation Neutron Source).

 Among the five people selected by The Minerals, Metals & Materials Society (TMS) for the 2011 Class of Fellows is ORNL's Steven Zinkle, who uses HFIR to study radiation effects on materials.

 Mike Simonson and John Katsaras have been named senior scientists in the Neutron Scattering Science Division

 Publication citations are needed for reports to our sponsor and for selection of annual report highlights. Send us the citation if your publication is not included on our lists. There is a standard acknowledgment for HFIR or SNS experiments. Let us know if research here contributed to your thesis.

 The National User Facility Organization reports that participants at U.S. national user facilities—such as synchrotron and neutron, nanoscience, high-energy and nuclear physics, microscopy, and astronomy facilities—now total more than 25,000.

From: [Ekkebus, Allen E.](#)
To: [Antonella Longo](#); [Cora Lind](#); [Eugenia Kharlampieva](#); [Greg Beaucage](#); [Malcolm Guthrie](#); [Michael K Crawford](#); [Patrick Woodward](#); [Peter Khalifah](#); [Stone, Matthew B.](#); [Sueng-Hun Lee](#); [Ursula](#)
Subject: Neutron scattering opportunities of interest
Date: Tuesday, April 12, 2011 7:11:55 AM

Dear all,

We would like to call your attention to two opportunities for neutron scatterers. The first event is a workshop in Oak Ridge directed to those new to the field and who wish to learn more about neutron scattering. The second opportunity allows comment to the National Research Council of Italy (CNR) on research infrastructure.

Al Ekkebus

What Can You Do With Neutrons?

A Workshop to Introduce Neutron Scattering Techniques to the Novice May 19-20, 2011, Oak Ridge National Laboratory

Clifford Shull and Bertram N. Brockhouse were awarded the 1994 Nobel Prize in Physics “*for pioneering contributions to the development of neutron scattering techniques.*” Today neutron scattering is a powerful suite of scientific tools for determining atomic and spin structure and dynamics and is widely used in condensed matter physics, materials science, materials chemistry, polymer science, biological sciences, and engineering. Neutron scattering experiments can be completed at a number of facilities spanning the globe, including the Spallation Neutron Source (SNS) and High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory (ORNL). Today the number of active neutron users in Europe outnumbers those that are active in the US, therefore there is a need to increase the number of neutron scattering users in the US to take advantage of the rapid growth in the capacity at the neutron scattering facilities in the US.

To address this challenge a Workshop will be held May 19 and 20 at Oak Ridge National Laboratory in the Joint Institute for Neutron Sciences. ***The goal of this workshop is to introduce the capabilities and opportunities of neutron scattering techniques to scientists with little or no neutron scattering experience.***

The meeting is designed to educate scientists interested in using neutron scattering in their research by:

- Presenting examples of scientific problems that have been solved by neutrons in determining hard and soft matter structure and dynamics
- Discussing the SNS and HFIR facilities and capabilities
- Detailing the process of writing a proposal to obtain neutron scattering time

- Elucidating the process of planning and executing an experiment
- Providing tours of SNS and HFIR

Breakout sessions will be held to allow one-on-one discussions of workshop participants with ORNL Instrument Scientists to identify how neutrons can be used to solve participants' scientific problems. These sessions will also include extensive panel discussions, with the goal of allowing all participants an opportunity to explore how they might apply neutron methods to address the challenges in their research. By the end of the Workshop, the attendees should have the vision and knowledge to prepare their own beamline proposal for performing experiments at the HFIR, SNS or other neutron facilities.

For more information, see the Web site at: [Neutron Workshop](#) or contact Hope Moore-Webb, Oak Ridge TN 865.576-8630; hmoore2@utk.edu. Funding for this workshop is provided by the Department of Energy, Office of Basic Energy Sciences, through the EPSCoR Grant, DE-FG02-08ER46528 and by the UT-ORNL Joint Institute for Neutron Sciences (JINS).

Opportunity for comment on Research Infrastructure

The National Research Council (CNR) of Italy is a public organization with the duty to carry out, promote, spread, transfer and improve research activities in the main sectors of knowledge growth and of its applications for the scientific, technological, economic and social development of the Country. CNR wishes to consult extensively the Italian community, stakeholders and international experts on the subject of Research Infrastructures (RI), with a distinction between "Large Research Infrastructures" (LRI) - e.g. synchrotrons, FEL neutrons, oceanographic ships, lasers facilities etc., and "Medium Research Infrastructures" (MRI) - e.g. analytical Facilities, lasers, NMR, etc.

The consultation is open at the web address www.cnr.it/questionario/. Through this consultation, your input will be sought on the future direction of the Italian Research Council. The consultation will also be used to refine a strategy document on RI, which will then form the basis for future spending and prioritization decisions made by the Council, and a framework for our consultation and advisory system. Feedbacks will be collated and analyzed at the end of the consultation and will help shape the RI strategies. The consultation process is open at the address www.cnr.it/questionario/ from 08:00 a.m. 4th April and will last [until 08:00 p.m. 1st July 2011](#). CNR greatly appreciates comments on the RI strategy and thanks you in advance for your assistance in helping us to shape our future.

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