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Welcome

Linda Horton, CNMS Director

Welcome to the inaugural issue of the CNMS User Newsletter! The path to this day has been inspirational. The growth of the CNMS has been phenomenal and exciting – from the ground-breaking ceremony in 2003 to the completion of the building in 2005 – and finally to growth of the user program to a vibrant, multidisciplinary community from academia, industry, and government laboratories. During the 2008 fiscal year, over 400 unique CNMS users worked at the CNMS, used our computing resources, or received materials synthesized at the CNMS. Our user group showed significant growth in international- and industry-based users.

The “vision” for CNMS as stated by our sponsor, Basic Energy Sciences of the Department of Energy (DOE), is to provide world-class user capabilities and to do world-leading science. The scientific program at the CNMS includes the research that you do here as a user and the in-house science program that our staff does independently of the user program. One goal of the in-house science program is to do the research that will keep you coming back to the CNMS – research that is on the forefront of nanoscience and the development of novel instrumentation, techniques, and software. Peter Cummings’ article in this newsletter discusses the outcome of our strategic planning to define the long term goals of this part of our program.

We are looking to you as users of the CNMS to help us insure that we have and continue to develop world-class user capabilities. Our challenge for the coming years is to further improve the quality of our program. The annual user survey provides some of the feedback that we need, but I would like to challenge you to provide more guidance. What equipment do we lack? How can we improve the research support you receive when you come to the CNMS? What exciting science would you like to do with us – but can’t? How can we improve our application/review processes? Training and safety are essential for continued operation of our user program – what suggestions do you have for improving the training that we provide? We will be engaging the Users’ Executive Committee in our planning processes. However, I welcome your independent input – my email is hortonll@ornl.gov.

On a final note, if you would like to have a presentation at your institution on the CNMS generally or a specific scientific area by one of our staff, please let us know. We would welcome the opportunity to visit your university, company, or laboratory.

Message from the UEC Chair

Yoke Khin Yap, Michigan Technological University

This inaugural newsletter has been put together by the first Users’ Executive Committee (UEC) elected in December 2007 (http://www.cnms.ornl.gov/uec/about_cnmsug.shtm). To facilitate the mission of the CNMS User Group to enhance the communication and understanding between users and CNMS, the UEC has created the following: 1) a new “CNMS User Group” domain in the official CNMS website, 2) a periodic newsletter, and 3) a partnership with CNMS in organizing the annual user meeting (September 24-26, 2008) - the major forum for current and potential users to present productive research in CNMS.

The UEC has also participated in other activities. As UEC Chair, I attended the CNMS Advisory Committee meeting January 2008. The meeting is an evaluation platform to improve CNMS capabilities for promoting high-impact collaboration with its user group. The UEC Chair is also a member of the National User Facility Organization (NUFO, <http://www.nufo.org/>). On April 10, 2008, NUFO sent letters to President Bush and the Majority Leader of the U.S. Senate to request that supplemental appropriations would include funding for scientific research and STEM (Science,

Technology, Engineering, Mathematics) education. On December 8, 2008, NUFO sent another letter to President-Elect Mr. Barack Obama for the same purpose. Last September, UEC members discussed and evaluated the conduct of our business. We have identified several measures to further improve collaboration between users and CNMS. The minutes of the UEC meeting and the user meeting will be posted online.

Questions and Suggestions: Users and potential users are encouraged to contact myself or any of the UEC members with questions and suggestions that you may have for productive collaboration with CNMS. We are also looking forward to hearing from you with your latest research breakthroughs conducted at CNMS (see solicitation herein). Let's work together to construct high-impact research at CNMS!

The Scientific Research Program of the Center for Nanophase Materials Sciences

Peter T. Cummings, CNMS Principal Scientist

The CNMS at Oak Ridge National Laboratory is a DOE user facility. This will come as no surprise to the readers of this newsletter. We currently serve about 400 users per year, associated with about 220 current user projects. However, the CNMS is also a scientific research center, with staff spending approximately half of their time pursuing research that is independent of the user program. As a center, we are evaluated by our sponsors (i.e., the Scientific User Facilities Division of the Office of Basic Energy Sciences, within the DOE Office of Science) both on our effectiveness as a user facility, and on the quality of our internal science program.

During 2007, Center Director Linda Horton and I held a series of meetings with staff, meeting with junior, mid-career and senior staff in separate groups, as well as research groups, in order to develop a strategic plan for the internal science research program of the CNMS. We also sought the input of our Advisory Committee and the User Executive Committee (UEC). Our strategic plan, which will evolve over time, is shaped by four important considerations in developing the themes for the internal research program:

1. **Addressing Nanoscience Grand Challenges.** First and foremost, the CNMS research themes are intended to address outstanding scientific challenges in nanoscience for which the CNMS has unique world-class scientific capabilities, reflected in the knowledge and expertise of our staff and our current and future instrumentation¹.
2. **Relationship to the CNMS User Program.** Our science themes must lead to novel capabilities that will serve our most demanding users now and in the future, attracting future users.
3. **Input from Stakeholders.** The CNMS internal science program will continue to be formulated in consultation with the Advisory Committee, the users as represented by the UEC, and the DOE BES.
4. **Unique "instruments" available at ORNL.** In addition to unique instrumentation at the CNMS, we have built the user program and internal science program to take advantage of unique capabilities/facilities across ORNL, such as the neutron scattering facilities [Spallation Neutron Source (SNS) and High Flux Isotope Reactor (HFIR)], the leadership-class computing facility in the National Center for Computational Sciences, and the BES-supported Shared Research Equipment user program, a key capability for nanoscience which emphasizes electron- and atom-probe microscopy and spectroscopy.

Out of this planning process, one overriding science focus emerged as the cornerstone of the CNMS internal research program: **Understanding, Designing, and Controlling the Dynamics and Spatial Aspects of Functionality in Nanoscale Systems.** This overall science focus is being addressed in three scientific themes:

- I. **Origins of Functionality at the Nanoscale.** Novel instrumentation and techniques to image and control functionality at the appropriate time, length, and energy scales lie at the heart of discovery of the new physics and chemistry emerging at the nanoscale. New tools built on current capabilities and new discoveries will be developed and used to understand nanoscale functionality and the interactions of nanoscale materials with larger assemblies.
- II. **Functional Polymer Architectures.** This theme focuses on advancing our fundamental understanding and control of polymer structure, dynamics, and function as controlled by weak forces and whose properties are largely dependent on interfacial nanoscale phenomena. These investigations are rooted in controlled synthesis of well-defined synthetic and bio-inspired polymers, and hybrid materials with rigorous characterization.
- III. **Understanding Emergent Behavior.** This research builds on the strong CNMS theoretical effort in this area, combined with experiments, focusing on understanding the emergence of collective behavior at every scale from the electronic structure to the mesoscale. This theme includes multiscale aspects of functionality in complex systems and assemblies of nanoscale materials such as oxides, as well as bio-inspired nanomaterials.

As a companion to these themes, the CNMS **Nanofabrication Research Laboratory** provides a cross-cutting capability whose research addresses the challenge of unraveling the properties of nanomaterials through their integration into systems with precisely defined functionality across multiple length and time scales.

¹In this context, instrumentation is intended to include not just experimental facilities, but also "instruments" for theory and modeling, including codes optimized to run on the leadership-class computing platforms.

In order to embrace the scientific themes organizationally, we restructured our research groups into five groups:

1. Nanomaterials Theory Institute
2. Macromolecular Nanomaterials
3. Multiscale Functionality
4. Imaging Functionality
5. Nanofabrication Research Laboratory

Group 1 is primarily identified with, and has leadership responsibility for, Theme III; group 2 is primarily identified with, and has leadership responsibility for, Theme II; groups 3 and 4 are primarily identified with, and have leadership responsibility for, Theme I; group 5 is cross-cutting to all of the themes.

The theme leaders for each of the research themes, as well as senior staff members from each theme, meet monthly to review progress on theme-based research, exchange ideas about new developments in the scientific literature and within the CNMS, and seek to find synergy between the themes to achieve the larger overall science focus. We are delivering exciting theme-related science on a daily basis at the CNMS. We invite you to learn more about this from the science highlights published on the CNMS web site, where we highlight both user research and theme-related research accomplishments (<http://www.cnms.ornl.gov/news/news.shtm>). Articles on each of the themes are also planned for forthcoming issues of this newsletter.

Staff Profiles

Each issue we will interview a couple of CNMS staff members for their insight into the facility and give readers a chance to find out what's going on. For this issue we interviewed Sergei Kalinin and Jamie Messman.

Sergei Kalinin

➤ **What is your research area?**

Scanning probe microscopy (SPM) and nanoscale electromechanics, including bias-induced phase transitions, and electromechanics of biological and molecular systems.

➤ **Where were you before coming to CNMS?**

Following a PhD at University of Pennsylvania supervised by Prof. Dawn A. Bonnell, I joined ORNL initially as a Eugene P. Wigner Fellow and subsequently a research staff scientist.

➤ **What attracted you to CNMS?**

SPM is by definition an interdisciplinary subject which requires technique (hardware and software) and theory development, accessibility and contact with materials synthesis and theory groups. CNMS allows us to combine the technique development and fundamental science under the framework of basic research, and application of the techniques and theoretical knowledge to a broad range of materials systems through user collaborations.

➤ **Which CNMS theme group do you work in?**

Group: Imaging Nanoscale Functionality; Theme: Origins of Functionality at the Nanoscale.

➤ **What are your duties at CNMS?**

Undertake research and coordinate user programs and match users to existing capabilities. Follow the research in the field and guide technique development aimed specifically at long lead-times (assuming that companies aim at medium- and short-term).

➤ **What are your current research interests?**

Coupling between electromechanical, electrical, and transport phenomena on the nanoscale in functional oxides and biological systems. Emergent phenomena in nanostructures, esp. transition metal oxides. Electrostatic and electromechanical interactions in liquids, biosystems, and molecular systems. Local probes of photoelectric phenomena in ferroelectrics, photovoltaic, and electroluminescent materials. Developing novel SPM techniques, mathematical analysis of SPM data, quantitative measurements of local properties by SPM.

➤ **Who are your research collaborators?**

Primarily strong theory groups (Anna Morozovska in Ukraine, Long Qing Chen at Penn State) and materials growth (Ramamoorthy Ramesh at Berkeley, Zuo-Guang Ye at Simon Fraser). Also, we have done a lot of work with Venkat Gopalan and Susan Troler-McKinstry of Penn State and Alexei Vertegel of Clemson.

➤ **What is your favorite aspect of working at CNMS?**

The CNMS provides a strong technical base, and a large number of technical specialists on one side and theorists on the other. I enjoy the ability to work with the leaders in the field through user programs and directly.

➤ **What equipment/techniques do you use at CNMS?**

Our group uses a number of techniques including, frequency dependent spatially resolved as well as band-excitation SPM, Scanning Gate Microscopy, Ultrasonic and acoustic force microscopy imaging.

➤ **What is your favorite recent research result?**

We have developed a pretty good understanding of mesoscopic polarization dynamics and polarization-defect interactions. Now we aim to extend this from the mesoscopic to the atomic level through interactions with electron microscopists and scattering experts at ORNL and Argonne.

Jamie Messman

➤ **What is your research area?**

Broadly, my research is in the area of synthesis and characterization of well-defined polymeric materials.

➤ **Where were you before coming to CNMS?**

I was a graduate student at The University of Southern Mississippi, under Professor Robson F. Storey. Immediately prior to my appointment at the CNMS, I was a post doctoral associate in the Chemical Sciences Division (CSD) at ORNL.

➤ **What attracted you to CNMS?**

The opportunity to conduct world-class research in an all-encompassing facility. The CNMS is a hot-bed of scientific diversity, which facilitates un-paralleled possibilities for collaborative research.

➤ **Which CNMS theme group do you work in?**

Macromolecular Nanomaterials group and Functional Polymer Architectures theme.

➤ **What are your duties at CNMS?**

I am a research chemist so my duties include small molecule and polymer synthesis and characterization. Since the CNMS is a user facility, I also spend time working closely with numerous collaborators to facilitate their research.

➤ **What are your current research interests?**

These revolve around how chemical composition and molecular and supramolecular architecture of stimuli-responsive polymers impact physical and chemical properties. We are working towards this through a thorough investigation of the synthesis and characterization of well-defined polymeric materials with selected functionality, composition, and molecular architecture. I'm interested in the response of certain polymers to external stimuli such as temperature, pH, solvent polarity and ionic strength in solution and on surfaces.

➤ **Who are your research collaborators?**

Collaborators in the last 12 months outside of ORNL include Tim Long (Virginia Tech), Brent Sumerlin (Southern Methodist U.), Charles McCormick and James Rawlins (Southern Mississippi), Lynn Loo (U. Texas, Austin and Princeton U.), James Hedrick and Charles Wade (IBM Almaden), Nikos Hadjichristidis (U. Athens, Greece), Apostolos Avgeropoulos (U. Ioannina, Greece), Patrick Geunoun (LIONS, Saclay, France), and Ting Xu (U. California, Berkeley).

➤ **What is your favourite aspect of working at CNMS?**

I don't know if I have a single favorite aspect of working at CNMS; there are too many. If I had to choose one aspect, it would be the team environment that we share in the group.

➤ **What equipment/techniques do you use at CNMS?**

As a synthetic polymer chemist, I use a plethora of synthetic techniques such as living anionic, controlled free radical, metallocene-catalyzed, controlled ring-opening, condensation, and cationic and anionic polymerizations. In addition, I utilize a full range of extensive set of polymer characterization tools available at the CNMS, plus the SNS facility next door.

➤ **What is your favorite recent research result?**

My favorite recent research results have been our findings related to a reactive polymer called poly(vinylidimethylazlactone) or PVDMA. The polymer (and monomer) are highly reactive toward nucleophiles, which is allowing us to generate interesting materials with specific properties: we can effectively modify the properties of PVDMA to respond to changes in temperature, salt, solvent polarity and ionic strength, as well as to light, all in one material. Also, we have recently found direct evidence of the controlled/living polymerization of amino acid N-carboxyanhydrides, a result which we are planning to submit to *Nature Materials*.

Science Highlights

One of the regular features of the CNMS user newsletter will be a section devoted to "Science News" which will include both short items on breaking research news like the one below, as well as more detailed research highlights from a number of research groups, together with announcements of interest. Some of the research highlights will mirror the CNMS News/Highlights web page, which provides information on recent achievements. However, we would also like to solicit CNMS users input for additional material describing current research interests and results, as well as any noteworthy announcements including relevant future conferences and meetings, positions available, academic comings and goings, etc. Research reports should be written as short articles and accessible to a wide yet informed readership (not just your peers) and include a short statement of the goals of the CNMS project together with who you are working with at CNMS. Further details and/or submissions should be sent to Sandy Lowe (lowes1@ornl.gov).

➤ **ORNL supercomputer simulation wins Gordon Bell Prize**

A team led by ORNL's Thomas Schulthess received the prestigious 2008 Association for Computing Machinery Gordon Bell Prize after attaining the fastest performance ever in a scientific supercomputing application. In addition to Schulthess, team members from CNMS included Gonzalo Alvarez, Paul Kent, Thomas Maier, Jeremy Meredith and Michael Summers. The team achieved a computing speed in excess of 1.3 petaflops in a simulation of a high-temperature superconductor using a version of a Dynamical Cluster Approximation code (DCA++) optimized for the

Cray XT5 Jaguar supercomputer at the National Center for Computational Sciences. The record-setting system performance enabled the team to include random disorder (impurities) in their simulations. CNMS users can now obtain access to Jaguar and the same DCA++ code to solve appropriate problems submitted via CNMS user proposals. For more information, see the ORNL press release http://www.ornl.gov/info/press_releases/get_press_release.cfm?ReleaseNumber=mr20081120-00 and the prize-winning research paper http://www2.computer.org/portal/c/document_library/get_file?folderId=97697&name=DLFE-3104.pdf.

Important Dates for your Calendar

- 2009 MRS Spring Meeting, San Francisco, California, April 13-17, 2009
- International Conference on Neutron Scattering, Knoxville, Tennessee, May 3-7, 2009
- [NSTI Nanotech 2009 Conference and Expo](#), Houston, Texas, May 3-7, 2009
- [National School on Neutron and X-ray Scattering](#), Argonne, Illinois and Oak Ridge, TN, May 30-June 13, 2009
- CNMS User Proposal deadline, May 2009 (specific date TBD)
- [International Symposium on Piezoresponse Force Microscopy](#) and Nanoscale Phenomena in Polar Materials (PFM – 2009), Aveiro, Portugal, June 23-27, 2009
- 2009 CNMS User Meeting and ORNL User Week, Oak Ridge, Tennessee, September 14-18, 2009 (tentative dates)

User Office Mailbox



This section of the newsletter is devoted to questions and answers about working at the CNMS and the user program in general. Please send your questions to cnmsuser@ornl.gov. Questions of general interest will appear in future issues of the newsletter, and we will collect all FAQs on the CNMS website as we receive them.

Does CNMS offer support for travel or local living expenses?

CNMS is not allowed to provide financial support for user travel. Travel support is allowed under some ORNL research programs, but generally requires that the travel will advance the Mission of the supporting program.

Where can I find information about lodging facilities nearby?

There are links to housing options on the CNMS web site; see "Working at CNMS" on the menu and click "Local Information". These are generally commercial chains, including extended-stay hotels. ORNL does not have on-site lodging at this time. ORNL is making plans to build an on-campus hotel adjacent to the CNMS and SNS at ORNL. Those plans have recently been delayed but this item is still high on the priority list for ORNL.

Are Foreign Nationals allowed to participate in research at the CNMS?

Access to ORNL and CNMS is permitted for Foreign Nationals. The lead time required to process a badge request depends upon the country of citizenship and/or birth. Currently lead times are 3-5 days for US Citizens, 15 days for Non-Sensitive Country Foreign Nationals, and 35-40 days for Sensitive Country Foreign Nationals. See the "Working at CNMS" web page for a list of countries designated as Sensitive. Unfortunately, due to US DOE requirements, badge requests from Foreign Nationals with a citizenship or birthplace in a country that is designated by the US Department of State as a state sponsor of terrorism cannot be processed within the term of a user project. See the "Working at CNMS" web page for additional details.

How do I add a new student (or collaborator) to an existing user project?

The Principal Investigator may request an additional collaborator be added to a user project by sending an e-mail to cnmsuser@ornl.gov. Include the name and e-mail address of the new collaborator as well as the CNMS project number in text. Any request to add a participant must be authorized by the Principal Investigator.

If you have news/comments/suggestions that you would like to share, send an email to cnmsuser@ornl.gov.