April 2013

CNMS User Newsletter

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Important Dates:
- Call for User Proposals: deadline is May 1
- ORNL User Week Aug. 12-16, 2013

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We encourage feedback and suggestions for the content of future newsletters. We are especially interested in receiving research highlights from CNMS users that may be featured in future issues of this newsletter. Please email us any time you have an important paper that is accepted for publication.

REMINDER! Proposal deadline is May 1 for new user projects that will start August 1.

Message from the UEC Chair

Anthony Hmelo, Vanderbilt University

University, government and industry scientists from around the world travel to ORNL to leverage the astounding array of equipment, facilities and expertise that makes the CNMS a leading center of excellence in nanoscience research. During my tenure on the User Executive Committee (UEC) since 2008 I have witnessed a breathtaking evolution of CNMS capabilities. As this year’s UEC Chair I am delighted to welcome prospective and current users of the CNMS to the current edition of our user newsletter, one of our primary means of communicating the important news, information and announcements of interest to our community.

The elected members of the UEC serve as your representatives in monthly conference calls with CNMS management where we discuss ways to improve your user experience. I encourage each of you to contact any member of the UEC with your ideas and suggestions so your voice may be heard. The minutes of our conference calls are openly available and archived for your reference on the CNMS web site. In addition I encourage everyone to make use of the CNMS Community Survey tool, also on the website which is always available for your use.

The UEC participates in planning our annual user meeting that showcases the exciting results and accomplishments we have achieved using CNMS resources. I encourage everyone to attend this year’s CNMS User Meeting during ORNL User Week in August.

Finally, we each have a vested interest in the success of the CNMS and this depends on the quality of the research that is performed here. I bring to everyone’s attention the open proposal call that is in progress with a submission deadline of May 1.

May this be a productive year and I look forward to seeing you around the CNMS!

-Tony
**CNMS 2013 User Executive Committee**

Chair (succession from Vice-Chair)– Tony Hmelo (Vanderbilt University)  
Vice-Chair—Vivek Prabhu (NIST)  
Secretary—Milan Buncick (Aegis Technologies Group)

At-Large Members –  
Nina Balke (ORNL/CNMS)  
Nazanin Bassiri-Gharb (Georgia Tech)  
Michael Hickner (Penn State)  
Marian (Molly) Kennedy (Clemson U.)  
Megan Robertson (U. Houston)  
Ichiro Takeuchi (U. Maryland)  
Rafael Verduzco (Rice U.)  
Past Chair, ex officio member: Martyn McLachlan (Imperial College, London)

**Proposal Calls**

**CNMS Call for User Proposals: High-Impact Nanoscience Research**  
**Deadline: Wednesday, May 1, 2013**

The Center for Nanophase Materials Sciences is soliciting proposals for user-initiated nanoscience research that will make effective use of CNMS facilities and staff expertise. The CNMS nanoscience research program provides users with access to a broad range of capabilities for nanomaterials design, synthesis, characterization, and theory/modeling/simulation, in order to carry out studies that will significantly advance our understanding of nanoscale phenomena and develop functional nanomaterials systems. Access is provided at no cost to users for research that is in the public domain and intended for publication in the open literature.

The submission deadline is Wednesday, May 1, 2013. Approved projects will be granted access to CNMS facilities during the period August 1, 2013 through July 31, 2014.

The CNMS website provides detailed descriptions of specific CNMS Research Capabilities that are offered to users. Prospective users are invited and strongly encouraged to contact CNMS staff members in the respective research areas to discuss their proposal ideas and learn more about the specific capabilities of interest to them.

**Opportunity to request beamtime for Neutron Scattering**

The CNMS is cooperating with ORNL's neutron scattering facilities to allow users to request neutron beamtime within a CNMS user proposal, **provided that the main part of the proposed work would be carried out at CNMS**. To request beamtime at one of ORNL's neutron facilities, CNMS users should attach the 2-page Neutron Scattering appendix with their CNMS proposal submission. The beamtime request will be reviewed concurrently with the CNMS proposal review. CNMS access for any proposal will still be based entirely on the CNMS’s standard peer-review process. A CNMS user whose beamtime request is declined will be welcome to submit a standalone proposal directly to the neutron user program in their next proposal call. CNMS user proposals submitted during this cycle may request neutron beamtime during the **experiment period that will begin in January 2014**. Note that if the primary thrust of the proposal is to obtain access to neutron scattering, prospective users must submit the proposal directly to the neutron scattering user program.
News from CNMS

2013A Proposal Call Results

For the 2013A Proposal Call, there were 161 proposals submitted and 101 were approved. There are also projects from prior cycles that requested extensions bringing our active project count to 268.

Postdoctoral Opportunities at the CNMS

The program is open to all qualified U.S. citizens and non-U.S. citizens. Visit the website for more information and links to view other opportunities at ORNL.

12th International Workshop on Piezoresponse Force Microscopy (PFM): Theory, Techniques, and Applications

This workshop, held March 4-7 at CNMS, provided an in-depth description of recent advances in PFM and offered laboratory demonstrations designed for advanced practitioners. This was the 12th in a series that started at ORNL in 2007 and has since become a mainstream ferroelectric conference. Twenty-four participants received hands-on experience with ORNL-developed band excitation and multidimensional tools, which introduced participants to the "big data" side of scanning probe microscopy. Ultimately, the workshop built a network of PFM specialists and promoted rapid dissemination of theoretical knowledge, experimental protocols, and novel technique development.
New equipment/capabilities

A new Maccor 4000 battery cycler is available for battery research. The system is equipped with a temperature chamber with accurate temperature control from -20 to 100 °C. The cycler has 24 channels that allow simultaneous testing of 24 cells. The instrument is part of the characterization tool suite in the Chemical Functionality Group and is available for this upcoming proposal call!

Contact: Dr. Chengdu Liang

CNMS in the news

Researchers at ORNL working on a CNMS user proposal have developed the first high-performance, nanostructured solid electrolyte for more energy-dense lithium-ion batteries to replace flammable ones. The work lead by Dr. Chengdu Liang from the Chemical Functionality Group at CNMS was the subject of several press releases. Some of news organizations that carried the report included:

- MIT Technology Review
- ScienceDaily
- ClimateWire
- PhysOrg
- R&D Magazine

ORNL researchers developed a nanoporous solid electrolyte (bottom left and in detail on right) from a solvated precursor (top left). The material conducts ions 1,000 times faster than its natural bulk form and enables more energy-dense lithium ion batteries.

User Spotlight

Evgheni Strelcov - Postdoctoral Researcher in the Imaging Functionality Group

“I’m interested in the metal-insulator transition and resistive switching materials that can be used for fabrication of memristors, transistors, switches and other highly-demanded components of modern electronic devices. It is absolutely fascinating to me to study how ionic motion in a material can bring about a several-orders-of-magnitude change in its conductance. It’s like pushing a small rock from the top of a mountain causing a snow avalanche to go rolling down the valley. And what’s interesting – this link between chemistry and physics can be investigated at the nanoscale using scanning probe microscopy. I guess, that’s what attracted me to the Imaging Functionality Group, where I currently am.”

Dr. Strelcov is a Postdoctoral Associate in the Imaging Functionality Group since 2011, mentored by Dr. S. V. Kalinin. He received his PhD in Applied Physics in 2011 from Southern Illinois University and MS degree in Inorganic Chemistry in 2004 from Moldova State University, Moldova. He has published about 20 papers and been recognized with several awards. Evgheni likes cats and is especially fond of fireplaces.


**CNMS Staff Science Highlight**

**Surface-Induced Orientation Control of CuPc Molecules for the Epitaxial Growth of Highly Ordered Organic Crystals on Graphene**

**Scientific Achievement**

Graphene was shown to direct the assembly of copper phthalocyanine (CuPc) molecules into epitaxially-aligned superstructures relevant to organic electronics. Theoretical modeling of the mechanisms responsible for this alignment revealed that van der Waals interactions and interfacial dipole interactions induced by charge transfer both play important roles.

**Significance**

Fundamental understanding of molecular interactions at interfaces is important to control the nanoscale morphology and orientation of organic semiconductors to improve optoelectronic processes for high-performance organic electronic devices. Here, graphene is demonstrated to effectively template CuPc molecules to nucleate, orient, and pack in the face-on orientation, the ideal structure for high-performance organic photovoltaics.

**Research Details**

- CuPc was thermally evaporated in high vacuum onto both as-grown graphene on Cu, and graphene transferred onto Si substrates.
- The nucleation, orientation and packing of CuPc molecules on films of graphene were investigated in a systematic experimental and theoretical investigation that combined X-ray scattering and diffraction, scanning probe microscopy, and electron microscopy with first-principles calculations.


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**SEM image of large 2D strip-like crystals of CuPc that are epitaxially aligned with the graphene surface and oriented along the graphene grain boundaries.**

(a) Theoretical modeling of CuPc molecules interactions with graphene in both face-on and side-on orientations (b) STM image of CuPc molecules aligned in the face-on orientation on graphene. Bottom left inset is a higher magnification STM image, top right inset schematically shows the molecular orientation.

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**CNMS Staff Spotlight**

**Mina Yoon** - *Staff member in the Nanomaterials Theory Institute*

“I am doing research in the field of theoretical and computational condensed matter physics. The primary focus of my research lies on understanding the fundamental principles of growth mechanisms, novel properties, electronic ground- and excited-state properties and functionalization of low-dimensional materials, such as surface-based materials, metal/oxide films and organic/inorganic/hybrid, oxide and carbon-based nanostructures. Especially, I am interested in the utilization of these materials for energy applications. I use various theoretical approaches including first-principles quantum mechanical and many-body potential approaches, continuum elasticity theory and microscopic and phenomenological modeling.

As a theoretician it is very exciting to work at CNMS where I have direct access to a large amount of in-house experimental data from the state-of-art instrumentation and techniques, which I use to validate my theoretical models. On the other hand, experiments very often depend on theory support to get a deeper understanding of the observed phenomena and to promote further development. Also, I very much like the international environment at ONRL with many opportunities of collaborating with researchers from all over the world.”
As a computational material scientist, I utilize various high-performance computer resources at CNMS and ORNL. My theoretical work is very much related to many experiments at ORNL that make use of pulsed laser deposition techniques, STM, HRTEM and other state-of-the-art experimental facilities.”

Dr. Mina Yoon is a theoretician at the NTI (Nanomaterials Theory Institute) working closely in collaboration with experimentalists of the Functional Hybrid Nanostructures group, the Imaging Functionality group and other groups at the center. Before coming to CNMS, she worked at ORNL’s Materials Science and Technology Division, was a research assistant professor at the Physics and Astronomy Department of the University of Tennessee and worked as Max Planck Fellow at the Fritz Haber Institute in Berlin, Germany. She received her Ph.D. degree in Theoretical Condensed Matter Physics in 2004 from Michigan State University and her M.S. degree in Physics in 1999 from Seoul National University, Korea.

CNMS Staff – Honors and Awards

The Center for Nanophase Materials Sciences' Nina Balke has been unanimously selected by the American Ceramic Society's board of directors to receive ACerS's Robert L. Coble Award for Young Scholars. Nina received an Office of Science early career research grant in 2011 to investigate the complex interplay of ionic and electronic transport in battery materials.

Congratulations Nina!