August 2015

CNMS User Newsletter

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Important Dates:

- CNMS User Meeting
  -September 1-2, 2015
  Registration Deadline: August 19
- 2016 UEC Election:
  -Nominations Open
  -Online Voting in October
- Call for Proposals
  -Deadline: October 21
  to be announced soon!

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Message from the CNMS Director

Dear CNMS users,

As CNMS is starting to look back on its 10-year history, and – more importantly – forward to its future, this year's user meeting is particularly important for us. I'm very pleased to see that the UEC has structured the meeting in a rather unusual format: The emphasis on discussions and short presentations will provide us with the type of feedback that we need. I am very much looking forward to the sessions in which you – as users – play the dominant role in identifying needs and opportunities. I encourage you to come prepared with ideas and suggestions, and hope you will be able to use the time at the meeting to interact with other users and to jointly express the most critical needs we can and must address. Unfortunately, no research center can do everything, nor will we ever be able to fulfil every wish. However, with the right feedback from the user community, we can focus on those areas that are most critically needed.

The user meeting also coincides with the nomination deadline for the User Executive Committee. It is hard to overstate the role of this committee – its members are the spokespersons of the users, and critically important advisors to the CNMS leadership team. If you feel that you have ideas and suggestions that would make CNMS even better, please consider offering your time and energy and play an active role in the UEC!

Finally, on a lighter note: We will once again hold a RidgeDance Film Festival during the User Meeting, and if you have short video clips or other visual material that represents your CNMS work, please contact Chris Rouleau at rouleaucm@ornl.gov. And, of course, don't forget that the registration deadline for the User Meeting is Wednesday, August 19!

Best regards – and see you soon!
Hans Christen

Upcoming Events

2015 User Meeting: September 1-2

Agenda and Abstract Booklet *now available!*

The Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory and its User Executive Committee are pleased to announce the CNMS User Meeting on September 1-2, 2015 with the theme of "Planning CNMS Science for Its 2nd Decade." This meeting will feature a set of forward-looking roundtable discussion sessions with the primary goal of collecting community input on future research directions and the consequent resource needs of current and future CNMS users.

Keynote addresses will be given by Tim Lodge (U. Minnesota) and Marco Buongiorno Nardelli (U. North Texas). Roundtable sessions are organized around five technical focus areas, including 24 invited speakers and more than 50 poster presentations. See the meeting website at http://www.cnms.ornl.gov/workshops/UM2015/index.shtml for a list of roundtable topics, speakers, and registration information. The registration deadline is **August 19** and advance registration is required.

Fall 2015 Call for User Proposals

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, October 21, 2015. Approved projects will be granted access to CNMS facilities during the period February 1, 2016 through January 31, 2017. 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.

*** It is important to use the latest version of the **CNMS Proposal Form** because the equipment offered is subject to change and only the latest form contains the up-to-date list.***

About the UEC
-Contact information
-Web links

News from CNMS

User Executive Committee Election

The Center for Nanophase Materials Sciences is seeking nominations of candidates to run for election to the 2016 CNMS User Executive Committee (UEC), which will be elected this fall by the users. The UEC is the principal voice of the CNMS user community and is expected to make recommendations to CNMS management on matters affecting the user community such as operating policies and needs for facilities, as well as leading planning for the annual User Meeting. The UEC consists of a Chair, Vice-Chair, Secretary and up to 7 At-Large members. We are currently seeking nominations for Vice-Chair, Secretary, and three At-Large positions to serve two-year terms. The members whose terms are expiring are Milan Buncick, Zheng Gai, Martyn McLachlan, and Ray Unocic.

Eligibility: All members of the CNMS User Group are eligible for election to the UEC and the current membership list is posted at www.cnms.ornl.gov/uec/CNMSUG_members_072415.pdf. Self-nomination is permissible and encouraged; also current members with expiring terms may be nominated to run for re-election. For additional information, see the User Group Charter.

To make a nomination: Send an email to cnms-uec@ornl.gov identifying the nominee(s) and the office(s) for which you are nominating them (Vice-Chair, Secretary, or At-Large). To expedite your nomination, it is strongly suggested that you identify another CNMS user who is willing to second the nomination, CC that member on your nominating email, and ask them to confirm their support by a reply to cnms-uec@ornl.gov. Nominations will be accepted through the end of the CNMS User Meeting on September 2, 2015.

Staff Updates

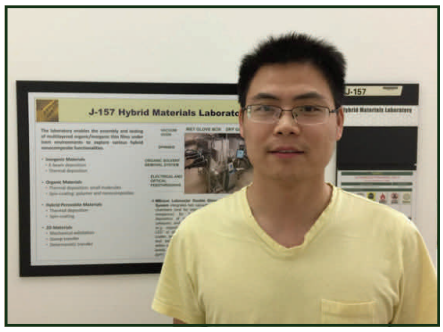
Michael Hickner, has joined the CNMS as the Group Leader for the Macromolecular Nanomaterials Group. Mike received his Ph.D. in Chemical Engineering from Virginia Tech in 2003. Before joining the Department of Materials Science and Engineering at Penn State in 2007, he was a postdoctoral researcher and then staff member at Sandia National Laboratories in Albuquerque, NM. Mike's research has focused on the synthesis and properties of ion-containing polymer membranes, measurement of water-polymer interactions using spectroscopic techniques, and the design of macromolecules to address challenges in green energy and clean water applications.

His work has been recognized by a Presidential Early Career Award for Scientists and Engineers in 2009 and led to over 120 peer-reviewed publications since 2001 that have been cited more than 6500 times.

Research Highlights

Bin Yang

Postdoctoral Fellow, Nanomaterials Synthesis and Functional Assembly Group
Center for Nanophase Materials Sciences

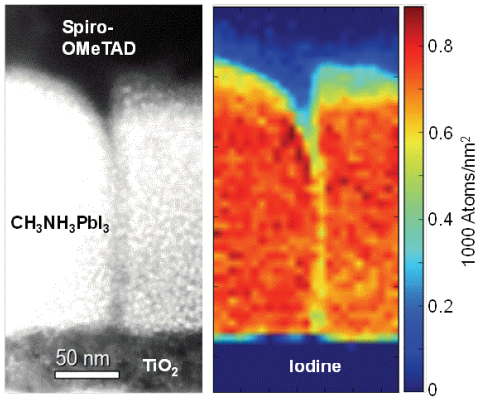


"I am interested in understanding of a broad range of fundamental properties including electronic, optical, and interfacial properties in materials spanning from organic semiconductors to nanostructured materials. My research mainly focuses on manipulating and utilizing the advanced electronic, optical, and interfacial properties of emerging organic/hybrid semiconductors and nanostructured materials to develop high-performance and cost-effective functional electronic devices such as solar cells, UV-visible-infrared photodetectors, x-ray sensors, thin film transistors, light emitting diodes, and memories. A variety of research equipment/techniques, such as x-ray scattering, neutron reflectivity/scattering, high resolution transmission electron microscopy, electron beam induced current mapping, electron energy loss spectroscopy, ultrafast laser spectroscopy, and Raman spectroscopy, are widely used in my studies. The reason that I chose CNMS to acquire postdoctoral training is because this place has highly collaborative and multidisciplinary research teams as well as the world-class research facilities covering a wide range of research areas including organic conjugated molecules, nanomaterials, oxides, as well as theoretical modeling."

Prior to joining CNMS, Dr. Bin Yang worked as a Research Assistant in the University of Nebraska-Lincoln. He obtained his Ph.D. degree in 2013 from the University of Nebraska-Lincoln, and the M.S. degree in 2010 from Hunan University, China.

Here's a recent highlight from Dr. Yang's research at CNMS that was published in the *Journal of the American Chemical Society.*

Activating Grain Boundaries in Perovskite Solar Cells



Cross-sectional TEM (left) and compositional analysis by electron energy loss spectroscopy (right) of a hybrid perovskite solar cell. By combining such data with electron beam induced current imaging (not shown), this study reveals how the vertical boundaries between single-crystalline perovskite grains can be activated with hole transport media to efficiently collect photogenerated charges.

This research was performed at the Center for Nanophase Materials Sciences.

Scientific Achievement

A new morphology for perovskite solar cells was realized that activates vertical grain boundaries between single-crystalline grains to enhance the collection and transport of photogenerated charges.

Significance and Impact

This discovery enables an industrially-scalable, cost-effective approach for producing highly-efficient hybrid perovskite solar cells with nearly 100% internal quantum efficiency.

Research Details

- A simple layer-by-layer fabrication process that includes air exposure leads to large single crystalline perovskite grains with vertically oriented grain boundaries.
- The hole-transport medium Spiro-OMeTAD infiltrated into the grain boundaries participates as carrier collector and forms transport channels.
- The prototype cells exhibit an average power conversion efficiency of ~ 16%.

B. Yang, et al. *J. Am. Chem. Soc.* **137** (29), 9210 (2015). DOI: 10.1021/jacs.5b03144

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THE UNIVERSITY of TENNESSEE KNOXVILLE

OAK RIDGE National Laboratory

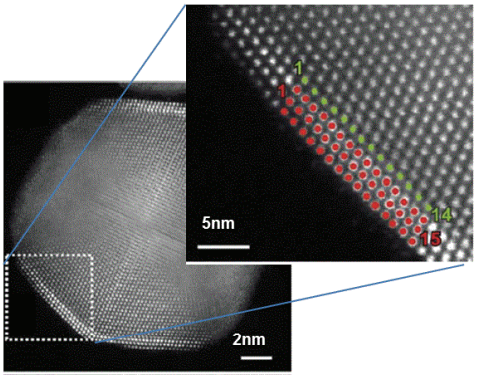
Younan Xia
Brock Family Chair and Georgia Research Alliance (GRA) Eminent Scholar in Nanomedicine
Georgia Institute of Technology

"My group's research focuses on designing novel approaches to the facile synthesis of colloidal metal nanocrystals with controlled sizes, shapes, structures, compositions, and properties, which did not exist previously. These novel nanocrystals open up a world of opportunities for many applications in plasmonics, sensing, electronics, photonics, photovoltaics, display, catalysis, fuel cells, and biomedical research, all of which will have a profound impact on the society. The CNMS is a world leader in research with cutting edge facilities, instruments, techniques, and experts all dedicated toward exploring and understanding fundamental scientific questions in current and emerging research areas. At the CNMS, we make extensive use of the aberration-corrected, high resolution TEM/STEM instruments, as well as their atomic resolution imaging, *in situ* heating, and elemental mapping (EDX and EELS) capabilities. The scientists who work at CNMS are all experts in their field, providing tremendous knowledge, skill, and scientific opinions on the work that we collaborate on with them. Their expertise is invaluable in not only designing experiments, but also in analyzing and understanding results and the data acquired. We are particularly grateful to the collaboration with Dr. Miaofang Chi on a number of exciting projects and to get interesting results for joint publications in high impact journals."

Professor Xia has co-authored more than 620 publications in peer-reviewed journals, has been cited more than 90,000 times, and has an h-index of 156. He received his B.S. degree in chemical physics from the University of Science and Technology of China (USTC) in 1987, a M.S. degree in inorganic chemistry from University of Pennsylvania with Professor Alan G. MacDiarmid in 1993, and a Ph.D. degree in physical chemistry from Harvard University with Professor George M. Whitesides in 1996.

Following is a highlight from Dr. Xia's user research in CNMS that was recently published in *Nature Communications*.

Quadrupling the Activity of Core-Shell Catalyst Particles



Transmission electron microscopy imagaes showing the morphology and atomic structure of typical Pd@$Pt_{2.7L}$ icosahedra nanoparticles

Scientific Achievement

Electron microscopy reveals that lattice distortions in Pd-Pt core-shell catalyst particles lead to four- to eight-fold enhancements in activity for oxygen reduction.

Significance and Impact

This discovery leads to a novel and effective synthesis approach for electrocatalysts with greatly enhanced activity and durability.

Research Details

- High-resolution STEM imaging revealed unique atomic structures with coexisting twin boundaries and strained core-shell arrangements, resulting in lateral confinement and compressive strains within Pt surface layers.
- Specific and mass activities toward the oxygen reduction ORR are enhanced 8X relative to a commercial Pd@Pt catalyst and after 10,000 cycles, mass activity is 4X higher than the commercial catalyst.

Work was performed as a User Project at the Center for Nanophase Materials Sciences, Georgia Institute of Technology, University of Wisconsin-Madison, and Xiamen University.

X. Wang, et. al., *Nature Communications*, 2015. DOI: 10.1038/ncomms8594.

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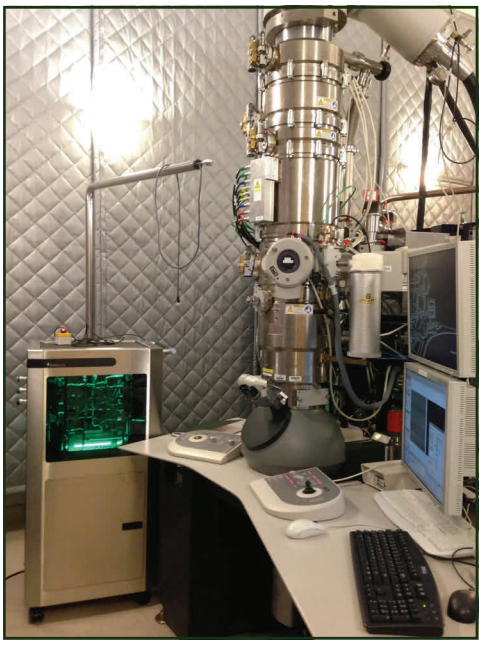
New Equipment



The FEI Titan aberration-corrected TEM/STEM has recently undergone a major upgrade to provide enhanced capabilities for analytical and *in-situ* microscopy. The upgrades include:

- Addition of a large active area (60mm2) EDAX silicon drift detector (SDD) for high-collection-efficiency energy dispersive X-ray spectroscopy (EDS) data acquisition. The Titan can now be used for the simultaneous acquisition of EDS and EELS spectrum images.
- Protochips *Atmosphere* gas environmental cell holder for conducting *in-situ* gas reactions at pressures to 1 atm. and temperatures up to 1000°C. This new holder complements other *in-situ* holders available for use on the Titan, including holders for electrochemistry/liquid-flow (Protochips *Poseidon*), electrical biasing and heating (Protochips *Aduro*), and *in-situ* atomic force microscopy (Nanofactory).
- Gatan *OneView* CMOS camera with *in-situ* option for high-frame-rate image/video capture (camera will be installed by September 30, 2015).

CNMS Honors and Awards

Peter Maksymovych is the 2015 winner of the Peter Mark Memorial Award of the AVS, which is awarded annually to a young scientist or engineer who has contributed outstanding theoretical or experimental work, at least part of which must have been published in an AVS Journal. Peter was cited "For high level frontier chemical and physical contributions to nanoscience."

Sergei Kalinin has been named a Fellow of AVS in recognition of sustained and outstanding scientific contributions in research and in particular "For development of revolutionary scanning probe microscopy techniques and application to transformative scientific discoveries in physics, chemistry, and materials sciences." Sergei is also a past recipient of the Peter Mark Memorial Award (2008).

Career Opportunities at CNMS

Visit the website for more information and links to view open positions as well as other opportunities at ORNL.

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.