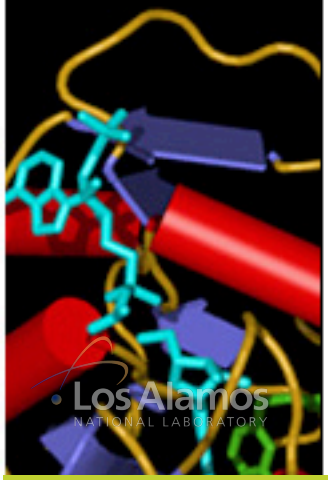
AOT & LANSCE The Pulse

June 2011

INSIDE






# Lujan Center user Ellen Moons receives Swedish national prize for scientific achievement

*King Carl VI Gustaf of Sweden presents Moons with the Göran Gustafsson Prize in physics.*
*Photo credit: Markus Marcetic/©KVA*

Lujan Neutron Scattering Center user Ellen Moons, associate professor of materials physics at Karlstad University in Sweden, was recently awarded the Göran Gustafsson Prize in physics for her achievements in furthering the development of organic and hybrid solar cells. The Göran Gustafsson prize is awarded annually by the Royal Swedish Academy of Sciences for outstanding scientific achievement in physics, chemistry, mathematics, medicine, and molecular biology. The prize, named after a Swedish businessman, is considered the most prestigious prize for young scientists in fundamental science disciplines at universities in Sweden. Moons will receive 4.5 million Swedish Crowns ($700,000) in research funding and a personal prize of $15,000. She plans to use part of the research grant for building a polymer solar cell device lab at Karlstad University. King Carl XVI Gustaf of Sweden presented Moons with the prize at an awards ceremony at the Royal Academy of Science in Stockholm.

Moons used the neutron Surface Profile Analysis Reflectometer (SPEAR) at the LANSCE Lujan Center to understand the properties of polymer-fullerene thin films used for light harvesting systems. In collaboration with Lujan scientist Jarek Majewski (LANSCE-LC), she studied bulk heterojunction structures, in which an electron-donating component intermingles with an electron-accepting component. This concept has proven its importance for low cost organic polymer/fullerene solar cells. In such a solar cell, an exciton is formed in the polymer upon absorption of light and is separated at the interface between polymer and fullerene into an electron and a hole. According to the model, the electron-accepting fullerene derivative transports the electron to the metal electrode, and the electrondonating polymer transports the hole to the indium tin oxide (ITO) electrode. The need for efficient absorption gives rise to criteria regarding the polymer material and the film thickness, while the optimal film morphology in the solar cell is a trade-off between the criteria for efficient charge generation and charge transport. Despite the significant body of research in the area of polymer-fullerene blends, the organization of these structures and the interplay between the fullerenes and the polymer is not fully understood. Due to the sensitivity to low-Z elements, neutron reflectometry provides an excellent tool to probe the structure of these systems.

# From Alex's Desk



Colleagues,

Let me first take this opportunity to congratulate Martha Zumbro as the new AOT Deputy Division Leader for operations. In addition to her qualifications, Martha knows LANSCE facilities very well. I'm looking forward to collaborating with her. Please join me in congratulating and welcoming Martha.

We have started a very busy summer here at the TA-53 mesa. The Rosenfest, led by Alan Hurd, was a great success. It featured an impressive list of speakers and participants with great talks about LANSCE in the past, present, and into the future with MaRIE. The LANSCE tour, organized by Leilani Conradson, Tanya Herrera, Lisa Padilla, Olivia Maes, and Jason Reano, with the assistance of great and enthusiastic tour guides, was also a great success—almost 400 participants—an impressive organization endeavor!

We have also recently announced the Rosen Scholar sabbatical (for more details, see lansce.lanl.gov/media/2011%20Rosen%20Scholar%20Call.pdf ). The Rosen Scholar fellowship is intended to attract visiting scholars to LANSCE in the fields of nuclear science, materials science, defense science or accelerator technology. The Rosen Scholar is reserved for individuals whose career accomplishments in fields of research covered by LANSCE facilities are recognized as outstanding by the scientific community and exemplifies the innovative and visionary qualities of Louis Rosen. The Rosen Scholar is expected to be resident at LANSCE and bring his/her scientific expertise to LANSCE as well as the broader Los Alamos scientific community. The position will support the Rosen Scholar at their current salary including relocation expenses for up to one year.

Even though we are having a bumpy start of the LANSCE User Programs, users are starting to show up, including a large collaborative team from ORNL-SNS, and J-PARC (Japan Proton Accelerator Research Complex ), where LANSCE, in particular WNR, continues to play a very important role investigating issues with the mercury targets.

**'We have started a very busy summer here at the TA-53 mesa.'**

Don't forget the LANSCE neutron school. The July 12-22 LANSCE Neutron Scattering School will feature as its main topic neutron scattering techniques and how they compliment other analytical methods in relation to energy and environmental issues. For additional information, visit lansce.lanl.gov/neutronschool/.

Thanks to the hard work of Elena Fernandez and many others our World Wide Web presence is up to date—and most importantly will be maintained. Please take a look as you have a chance. As you know the Web presence is a very important component of an international user facility. I'm glad we're getting there. As always, your feedback is paramount.

On a safety note, with the beginning of the run cycle, the TA-53 mesa population will increase. Please be courteous; slow down when driving. I continue to witness excess speeds, in particular at La Mesita Road. Please be careful, and please make sure to stop for pedestrians. In addition, be alert of suspicious activities, in particular late at night and during the weekend. If possible, write the license plate number and contact the LANSCE Control Room at 7-5729 and 911 depending upon the situation. Bottom line, however, do not try to resolve the situation.

Last but not least, I'm taking this opportunity to also congratulate Ginger Grant for her 27 years at LANL, and her dedication to LANSCE since 1997. Ginger is retiring July 1. Please join me in wishing Ginger all the best and a lot of fun.

*LANSCE Deputy Division Leader Alex Lacerda*

# Collaboration meeting on fission measurements

Los Alamos and Lawrence Livermore National Laboratories (LLNL), and other national laboratories and universities, are collaborating on a major experimental effort to measure the fundamental fission properties that govern nuclear weapons and nuclear reactors. The goals of these projects are (1) to reduce the uncertainties in the fission cross section for plutonium-239 and uranium-235 to less than 1% and, (2) to measure the neutron output spectra in energy regions that have not been previously measured.

LLNL leads the development of a Time-Projection Chamber to obtain the required precision in the cross section measurement. To measure the neutron output spectra, LANL leads the effort to develop a new neutron detector array (Chi Nu) for both low and high energy neutrons. The experiments are performed at LANSCE's Weapons Neutron Research facility.

Approximately 50 collaborators gathered for a two-day meeting at LLNL to review the status of these efforts, discuss emerging issues and concerns, and to develop plans to achieve important milestones and complete these projects. This was the second meeting of this group; the first meeting took place a year ago at LANL. The LANL and LLNL Campaign-1 program managers and the DOE Nuclear Energy program manager described the importance of these measurements to their respective programs. Bob Haight (Neutron and Nuclear Science, LANSCE-NS) presented the status of the Chi Nu experiment. Experimenters described the status of their particular responsibilities and the theoretical basis for these measurements. Mark Chadwick (Computational Physics, XCP-DO) discussed how the data will be incorporated into the Nuclear Weapons design codes. The work supports the Laboratory's Nuclear Deterrence and Energy Security mission areas and the Science of Signatures and Information and Knowledge Science capabilities.

*LANSCE-NS postdoctoral researcher Hye-Young Lee presents the results of testing lithium-6 glass detectors.*

*XCP Division Leader Mark Chadwick describes how the results of the experiments will be incorporated into the weapons design codes.*

# Majewski to give lectures commemorating anniversary of Marie Curie's Nobel Prize

LANSCE-LC scientist Jarek Majewski has been invited to give a series of lectures at the Faculty of Chemistry University of Marie Curie-Sklodowska (UMCS) in Lublin, Poland to commemorate the centennial of the physicist-chemist's second Nobel Prize for "the discovery of the elements radium and polonium."

The faculty of chemistry of the UMCS and its Department of Interfacial Phenomena is the leading Polish scientific center to study interfaces, surface properties and colloidal science. Majewski's 10 lectures will discuss novel methods (including neutron and synchrotron scattering) to investigate structural and dynamical properties of soft condensed surfaces and ultra-thin structures, such as lipid membranes and Langmuir monolayers. These structures are biologically relevant models.

Majewski earned his master's degree in physics at Warsaw University in Poland and his doctorate at the Weizmann Institute of Science, Israel. He joined Los Alamos as a Director's funded postdoctoral researcher in 1995. He is an American Physical Society Fellow, adjunct professor at University of California, Davis, and author of more than 140 peer-reviewed papers in the area of soft-condensed interfacial science.

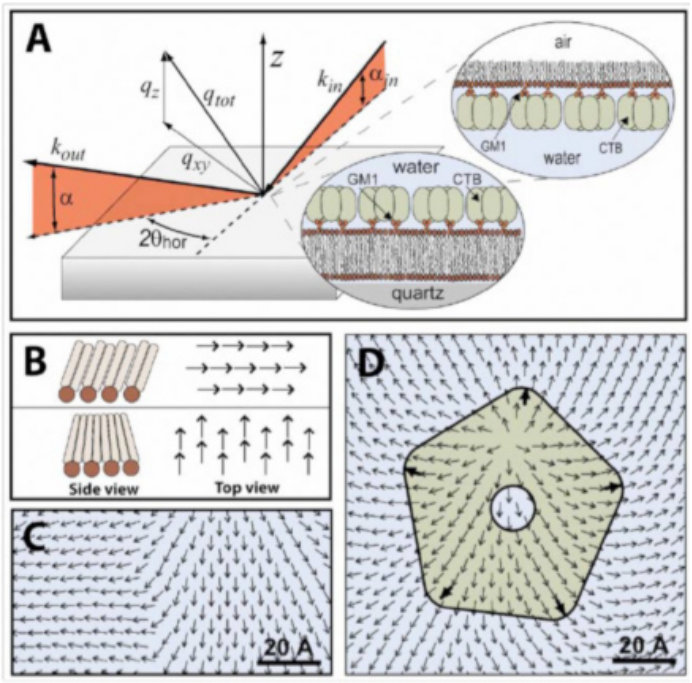
Marie Curie (neé Sklodowska), two times Nobel Prize laureate, was born in Poland. This year is the centennial anniversary of her second Nobel award.

# Cholera toxin binding to model membranes reveals potential signaling pathway

Biological membranes are complex, self-organized structures that define boundaries and compartmentalize space in living matter. Composed of a wide variety of lipid and protein molecules, these responsive surfaces mediate transmembrane signaling and material transport within the cell and with its environment. Interactions between proteins and the cell membrane are integral aspects of many biological processes. Diverse protein-lipid complexes exist including transmembrane proteins, peripheral membrane proteins, and proteins bound to membrane associated receptor molecules. The interplay between these biological components is multifaceted. Lipids can influence the structure and function of membrane proteins and at the same time, membrane proteins can impact lipid organization. These interactions can have an impact on the intake of toxins into cells.

LANSCE-LC scientist Jarek Majewski, in collaboration with the group of Professor Kuhl (University of California, Davis), used synchrotron x-ray scattering techniques to examine molecular level changes in lipid model membrane organization induced by multivalent binding of the cholera toxin B subunit (CTB). The cholera toxin selectively binds to ganglioside glycolipids in the membrane. Therefore, the scientists studied structural changes to the model lipid membranes before and after specific binding of cholera toxin to membrane-embedded ganglioside GM1 receptors. With unprecedented molecular details, the researchers showed how protein binding perturbed lipid packing, resulting in topological defects and the emergence of a new textured lipid phase (see figure). These altered packing arrangements are transmitted from the receptor-laden leaflet to the inner leaflet of the membrane, providing a means for outside-in signaling. Generation of such new lipid phases in membranes may have broad biological implications if perturbations to lipid order can be appropriated as a signaling mechanism by the cell and allow for new types of lateral heterogeneity in membranes. The textured domains provide a means for protein binding induced changes in lipid order to be spread laterally by cooperative self-organization of adjacent lipids. Resulting alterations of membrane structure may facilitate lipid domain clustering and potentially influence protein function. The researchers suggest that the formation of textured lipid microdomains via the multivalent binding of cholera toxin and protein aggregation into clusters are important in triggering the endocytotic pathway to bring the cholera toxin into the cell.

Reference: "Membrane Texture Induced by Specific Protein Binding and Receptor Clustering: Active Roles for Lipids in Cellular Function," *Proceedings of the National Academy of Sciences*,




*(A) The grazing incidence x-ray diffraction scattering geometry is shown with schematic insets representing the monolayer and bilayer lipid-cholera toxin B subunit (CTB) systems studied. qz = 2π sin α is the momentum transfer of diffracted x-rays normal to the interface and qxy = 4π sin θ is the momentum transfer perpendicular to the interface. (B) Tilt directors are vectors pointing along the lipids' alkyl chain backbones from the head group to the methyl end. (C) A boundary between two orientations of the lipid tilt director field. (D) Perturbation to the lipid tilt director field and associated topological defect induced by pentavalent binding of a single CTB protein.*

published online ahead of print; doi:10.1073/pnas.1014579108. This research benefited from the use of the Lujan Neutron Scattering Center at LANSCE, funded by the DOE Office of Basic Energy. The work supports the Laboratory's Science of Signatures capability.

# Neutron diffraction study of γ-chymotrypsin at the Protein Crystallography Station

Brandeis University graduate student Louis Lazar, his university colleagues, and researchers at the Protein Crystallography Station at LANSCE have collected the first complete neutron diffraction data set of γ-chymotrypsin at a spallation neutron source. Their goal is to develop methods for improving protein models with respect to hydrogen atom placement, such that the models might be better used in various computational methods that critically depend upon accurate and precise placement of hydrogen (H) atoms. In the field of rational drug design, significant improvements in the scoring functions of programs for computational ligand docking are possible when hydrogen sites can be explicitly assigned.

*continued on page 5*

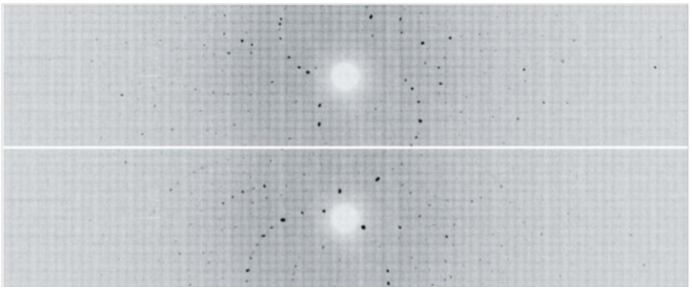
***Diffraction . . .*** In a protein, hydrogen is perhaps the most important atom, being involved in all aspects of enzymatic catalysis, drug binding, protein folding, dynamics, and protein engineering. Computational methods – such as *in silico* drug design and docking, as well as quantum mechanics/molecular modeling (QM/MM) – depend on accurate H-atom position data. Little experimental data are available, and these methods rely on idealized geometry and standardized libraries to infer the location of the H atoms. This can lead to inaccurate modeling and incorrect drug binding docking studies.

To address this critical knowledge gap, the scientists are generating neutron structures of γ-chymotrypsin prepared at various pHs to observe the changes in H bonding and H atom positions. Chymotrypsin is a biologically important molecule because it catalyzes the hydrolysis of proteins, degrading them into smaller molecules called peptides. Peptides are further split into free amino acids. The scientists subjected the γ-chymotrypsin crystal to hydrogen/deuterium exchange to enhance the neutron scattering imaging.

Initial data analysis reveals significant nuclear density for catalytically important residues. The researchers observed that the catalytic histidine is doubly protonated (deuterated). The serine and aspartate that make up the remainder of the catalytic triad do not show density for the presence of deuterium. The scientists also observed deuteration of backbone NH at terminal positions of beta sheets. Sample size and length of time to acquire neutron data are major impediments in the accessibility of neutrons to most structural biologists. However, these researchers obtained a complete neutron data set from a medium-sized crystal in under two weeks. These data will reveal many important details about the γ-chymotrypsin active site, ionization states of specific residues, as well as the hydrogen bonding patterns in the active site that support catalysis.

Los Alamos participants include Zoë Fisher, Andrey Kovalevsky, and Paul Langan (Bioenergy and Environmental Science, B-8). Brandeis University participants include Lazar, Dagmar Ringe, Greg Petsko, Aaron Moulin, and Walter Novak. The DOE Office of Science, Office of Biological and Environmental Research funds the Protein Crystallography Center and the Los Alamos scientists.

Reference: "Time-of-flight Neutron Diffraction Study of Bovine γ-Chymotrypsin at the Protein Crystallography Station," *Acta Crystallographica* **F67**, 587 (2011). The work supports LANL's Science of Signatures capability.



*Neutron Laue time-of-flight diffraction images of γ-chymotrypsin collected at the Protein Crystallography Station at two different ϕ settings at k = 30o and 90 o. For this representation, the time-of-flight data were overlaid to produce a conventional Laue pattern.*

# HeadsUP!

## Review foreign nationals host and co-host responsibilities

Hosts of foreign nationals should regularly review the list of responsibilities to ensure that they stay in compliance with DOE and LANL policies. See host and co-host responsibilities at int.lanl.gov/security/isec/fva/hosts.shtml. Contact OCI/FV&A at 665-1572 or 665-5561 if you have questions or concerns about your obligations as a responsible host or co-host.

## *Celebrating service*

Congratulations to the following LANSCE and AOT Division employees celebrating service anniversaries this month:

| | |
|---|---|
| Joseph Raybun, AOT-MDE | 35 years |
| Andy Steck, AOT-RFE | 30 years |
| Stephen Wender, LANSCE-NS | 30 years |
| Gary Cooper, LANSCE-LC | 25 years |
| James Knudson, AOT-OPS | 25 years |
| David Bell, AOT-OPS | 20 years |
| Karen Young, AOT-RFE | 20 years |
| Alex Lacerda, LANSCE-DO | 15 years |
| Mark Prokop, AOT-RFE | 10 years |
| Scott Baily, AOT-IC | 5 years |
| Jenay Vigil, AOT-ABS | 5 years |

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