

## **Materials Research Society (MRS)**

**PI: J. Ardie Dillen, Director of Finance and Administration, MRS**

**Performance Period: 5/15/2014 – 12/31/2014**

### **FINAL REPORT FOR DOE GRANT DE-SC0011650**

American Conference on Neutron Scattering (ACNS 2014) June 1-5, 2014 / Knoxville TN, USA <http://www.mrs.org/acns-2014/>

#### **Conference Highlights**

Scientists from the around the world converged in Knoxville, TN to have share ideas, present technical information and contribute to the advancement of neutron scattering. Featuring over 400 oral/poster presentations, ACNS 2014 offered a strong program of plenary, invited and contributed talks and poster sessions covering topics in soft condensed matter, hard condensed matter, biology, chemistry, energy and engineering applications in neutron physics – confirming the great diversity of science that is enabled by neutron scattering.

#### **Tutorials**

Two tutorials were offered, free to conference attendees. Featured topics were:

- Introduction to Rietveld Methods and Total Scattering to Analyze Powder Diffraction Data
  - Neutron powder diffraction is a widely used tool for structural characterization of a diverse range of materials including superconductors and energy storage materials such as batteries, solid oxide fuel cells, zeolites, ferroelectrics, etc. Neutrons provide unique sensitivity to light atoms and isotopes and enable non- destructive studies of large samples and samples within special environments. Application of total (Bragg and diffuse) scattering methods to powder materials provided access to local defects and disorder that drive many functional properties.
  - The aim of this tutorial was to give members of the powder user community an (1) introduction to neutron powder diffraction, and (2) introduction to total scattering methods and (3) hands on Rietveld analysis and PDF refinement of data collected at POWGEN (SNS) and NPDF (LANL).
- Real-Space Atomistic Modeling of Neutron Data Using SASSIE
  - This tutorial covered an introduction to molecular simulation methods to model neutron scattering small-angle and reflectivity data. This included a basic introduction to simulation methods and involved hands-on training in small groups to investigate common structural biology problems addressed using SASSIE.
  - Attendees who brought their own laptop were able to work through the lab section of the tutorial by using a web-browser.

The conference culminated with a free tour of the Oak Ridge National Laboratory (ORNL) facility.

#### **DOE Funds**

Limited travel support in the form of student reimbursement for the meeting registration fee and partial travel expenses were available for students who submitted an abstract to ACNS 2014. During the process of submitting abstracts, students were instructed to request travel support. Only the presenting author was considered for travel support (students and early career researchers only). The \$30,000 provided by DOE was allocated to 50 students and early career researchers at \$600.00 each:

Wolfgang Black  
Jeffrey Breidgan  
Adrian Brugger  
Zhikun Cai  
Michelle Calabrese  
Jeremy Carlo  
Bilin Chen  
Gurpreet Dhindsa  
Tyler Fears  
Richard Gillams  
Paul Godfrin  
Sanju Gupta  
Eli Heintzman  
Dennis Kim  
Harrison Knoll  
Abhishek Jaiswal  
Andrew Johnson  
Brian Kitchen  
Natalie Krzyzanowski  
Amber Larson  
Fankang Li  
Ke Li  
Bing Li  
Gong Li  
Philippe Lorchat  
Nicholas Martinez  
Luri Middleton  
Andrew Miskowiec  
Ryan Morrow  
Ngoc Nguyen  
Naresht Osti  
Trong Pham  
Carson Price  
Richard Roberts  
John Schneeloch  
Hao Shen  
Hillary Smith  
Charlezetta Stokes  
Wei-Shao Tung  
Kurt Van Delinder  
Mayme Van Meyeren  
Krishnamurthy Vemuru  
Karsten Vogtt  
Bo Wang  
Yuxing Wang  
Sidath Wijesinghe  
Minzhong Xu  
Fei-Chi Yang  
Zhenzhen Yu  
Mengze Zhu

**Plenary and Invited Speakers**

Young Lee, Massachusetts Institute of Technology  
Cevdet Noyan, Columbia University  
Darrin Pochan, University of Delaware

### Sources, Instrumentation and Software

Ben Frandsen, Columbia University  
Ken Herwig, Oak Ridge National Laboratory  
Boris Khaykovich, Massachusetts Institute of Technology  
Chuck Majkrzak, National Institute of Standards and Technology  
Steve Parnell, Indiana University  
Hard Condensed Matter  
Xianglin Ke, Michigan State University  
Young-June Kim, University of Toronto  
Israel Klich, University of Virginia  
Kathryn Krycka, National Institute of Standards and Technology  
Martin Mourigal, Johns Hopkins University  
Daniel Phelan, University of Minnesota  
Yuri Suzuki, Stanford University  
Stephen D. Wilson, Boston College  
Chenglin Zhang, University of Tennessee

### Soft Matter

Jerry L. Atwood, University of Missouri  
Wei-Ren Chen, Oak Ridge National Laboratory  
Michael Crawford, Dupont  
Matt Helgeson, University of California, Santa Barbara  
Ann Junghans, Los Alamos National Laboratory  
Norman J. Wagner, University of Delaware

### Biology

Julian Chen, Los Alamos National Laboratory  
Xiaolin Cheng, Oak Ridge National Laboratory  
Hirsh Nanda, National Institute of Standards and Technology  
Jonathan Nickels, Oak Ridge National Laboratory  
Mu-Ping Nieh, University of Connecticut  
Materials Chemistry and Materials for Energy  
Steven DeCaluwe, Colorado School of Mines  
Olivier Delaire, Oak Ridge National Laboratory  
Steven MacIntosh, Lehigh University  
James Neilson, Colorado State University  
Efrain Rodriguez, University of Maryland  
Nancy Ross, Virginia Tech  
Daniel Shoemaker, University of Illinois  
Engineering and Industrial Applications  
Levente Balogh, Queen's University, Canada  
Lynann Clapham, Queen's University, Canada  
Aaron Stebner, Colorado School of Mines

### Neutron Physics

Scott Dewey, National Institute of Standards and Technology  
Nadia Fomin, University of Tennessee

### Satellite Meetings

Magnetic Structure Determination from Neutron Diffraction Data June 5-8, 2014

See <http://neutrons.ornl.gov/conf/2014/magstr/> for more information.

The Magnetic Structure Determination Workshop aimed to enhance the community studying magnetism in materials by learning from experts the essential theoretical foundations to magnetic representation analysis and work through real examples to gain experience in solving and refining magnetic structures from neutron powder and single crystal diffraction data. Lectures and tutorial sessions covered:

1. Symmetry analysis using representation theory and the SARAh program.
2. Refinement strategies using the Fullprof Suite.
3. Magnetic structure determination from powder (constant wavelength and time-of-flight data) and single crystal data (constant wavelength)
4. Simulated annealing approach for structure solution.

The Magnetic Structure Determination Workshop 2014 was a satellite meeting of the ACNS 2014 Conference. Questions about this workshop can be sent to [Clarina de la Cruz](#) or [Ovi Garlea](#).

Ultra-Small-Angle Scattering Workshop (USAS-2014) June 5-6, 2014

*Please see <https://neutrons.ornl.gov/conf/usas2014/> for more information.*

The USAS-2014 Workshop was held at the Oak Ridge National Laboratory (on-site) on June 5 (afternoon session) and June 6 (full-day session). The workshop was organized as a satellite meeting to the ACNS 2014 Conference.

USAS-2014 was mainly focused toward user community updates and developments; therefore, the workshop program highlighted the latest interesting USANS/SANS and USAXS structural studies of condensed materials. The latest achievements in the USANS/USAXS instrumentation and sample environment techniques for USAS investigations were discussed. In addition, new interesting proposals for USANS/SANS studies and important scientific problems, which can be solved with contemporary USANS/SANS and USAXS techniques, were discussed at a special session of USAS-2014.

### **Poster Winners**

Sunday, June 1 (HP1.01)

T.C. McClanahan (photo not available)

*Experimental Validation of the SNS Sample Activation Calculator*

T. C. McClanahan<sup>1</sup>, E. B. Iverson<sup>1</sup>, F. X. Gallmeier<sup>1</sup>, M. B.R. Smith<sup>1</sup>

1. Neutronics Analysis, Oak Ridge National Laboratory, Oak Ridge, TN, United States.

Monday, June 2 (BP2.01)

Tianhao Wang

*Novel Non-Adiabatic Spin Flipper and Spherical Neutron Polarimeter Using High T<sub>c</sub> YBCO Films*



Tianhao Wang<sup>1</sup>, Steven Parnell<sup>1</sup>, Fankang Li<sup>1</sup>, William Hamilton<sup>2</sup>, Helmet Kaiser<sup>3</sup>, David Baxter<sup>1</sup>, Roger Pynn<sup>1, 2</sup>

1. Center for the Exploration of Energy and Matter, Indiana University, Bloomington, IN, United States.

2. Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, TN, United States.

3. University of Missouri Research Reactor Center, University of Missouri, Columbia, MO, United States.

Tuesday, June 3 (EP3.04)

Paul Godfrin

*Scattering Study of Reversible Cluster Formation in Concentrated Monoclonal Antibody Formulations*



Paul Douglas Godfrin<sup>1</sup>, Steven D. Hudson<sup>2</sup>, Isidro E. Zarraga<sup>3</sup>, Kunlun Hong<sup>4</sup>, Lionel Porcar<sup>5</sup>, Peter Falus<sup>6</sup>, Norman J. Wagner<sup>1</sup>, Yun Liu<sup>7,1</sup>

1. Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, United States.
2. Materials Measurement Laboratory, NIST, Gaithersburg, MD, United States.
3. Late Stage Pharmaceutical Development, Genentech Inc., South San Francisco, CA, United States.
4. Center for Nanophase Materials and Sciences, ORNL, Oak Ridge, TN, United States.
5. Large Scale Structures, ILL, Grenoble, France.
6. Time of Flight and High Resolution Group, ILL, Grenoble, France.
7. Center for Neutron Science, NIST, Gaithersburg, MD, United States.

Wednesday, June 4 (CP4.06)

Dennis Kim

*Phonon Anharmonicity in Silicon*



Dennis Sungtae Kim<sup>1</sup>, Hillary L. Smith<sup>1</sup>, Jennifer L. Niedziela<sup>2</sup>, Doug L. Abernathy<sup>3</sup>, Brent T. Fultz<sup>1</sup>

1. Applied Physics and Materials Science, California Institute of Technology, Pasadena, CA, United States.
2. Instrument and Source Division, Oak Ridge National Laboratory, Oak Ridge, TN, United States.
3. Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN, United States.

# A: Plenary & Prize Session

SESSION A4: Prize Lecture / Outstanding Student Prizes Announced  
Session Chairs: Julie Borchers and Stephan Rosenkranz  
Thursday Morning, June 5, 2014  
Summit I

\* Invited paper

SESSION A1: Plenary/Prize Lectures  
Session Chairs: Julie Borchers, Stephan Rosenkranz and Michael Kent  
Monday Morning, June 2, 2014  
Summit I

**8:00 AM Welcome and Introductions by Julie Borchers, Stephan Rosenkranz and Oak Ridge National Laboratory Representative**

**8:20 AM \*A1.01**  
**SHULL PRIZE WINNER: A Personal Retrospective of Neutron Scattering in Condensed Matter: From Magnets and Superconductors to Fractals and Films** Sunil K. Sinha, Department of Physics, University of California, San Diego, La Jolla, California.

**9:10 AM \*A1.02**  
**PLENARY: Material Construction through Peptide or Block Copolymer Solution Assembly with Kinetic Control** Darrin Pochan, Materials Science and Engineering Department, University of Delaware, Newark, Delaware.

**9:45 AM BREAK**

SESSION A2: Prize/Plenary Lectures: Award Presentation and Introduction of Fellows  
Session Chair: Stephan Rosenkranz  
Tuesday Morning, June 3, 2014  
Summit I

**8:15 AM Introduction of NSSA Fellows**

**8:35 AM \*A2.01**  
**SUSTAINED RESEARCH PRIZE WINNER: The Nature of Magnetism in Manganites and Superconductors** Jeffrey W. Lynn, NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland.

**9:10 AM \*A2.02**  
**OUTSTANDING STUDENT RESEARCH PRIZE WINNER: Towards Emergent Electrodynamics in a Geometrically Frustrated Magnet** Kate A. Ross, <sup>1</sup>Institute for Quantum Matter, Johns Hopkins University, Baltimore, Maryland; <sup>2</sup>NCNR, NIST, Gaithersburg, Maryland.

**9:45 AM BREAK**

SESSION A3: Plenary Lectures  
Session Chair: Patrick Woodward  
Wednesday Morning, June 4, 2014  
Summit I

**8:45 AM \*A3.01**  
**PLENARY: The Secret Lives of Quantum Materials: Case Studies Using Neutrons** Young Lcc, Department of Physics, MIT, Cambridge, Massachusetts.

**9:15 AM \*A3.02**  
**PLENARY: A Novel Application of Neutron Diffraction to National Infrastructure Remediation: Measurement of Stress Partitioning in Suspension Bridge Cables** I. C. Noyan<sup>1</sup>, Adrian Brugger<sup>2</sup>, Raimondo Betti<sup>2</sup>, Bjorn Clausen<sup>3</sup> and Donald W. Brown<sup>3</sup>; <sup>1</sup>Dept. of Applied Physics and Applied Mathematics, Columbia University, New York, New York; <sup>2</sup>Dept. of Civil Eng. & Eng. Mechanics, Columbia University, New York, New York; <sup>3</sup>Lujan Center, Los Alamos National Laboratory, Los Alamos, New Mexico.

**9:45 AM BREAK**

**8:25 AM Outstanding Student Prizes Announced**

**8:40 AM \*A4.01**  
**SCIENCE PRIZE WINNER: Tracking Atomic Structure Footprints of Broken Symmetry States** Emil Bozin, Brookhaven National Laboratory, Upton, New York.

**9:15 AM BREAK**

# B: Sources, Instrumentation and Software

SESSION B1: Instrumentation I  
Session Chair: Lee Robertson  
Monday Morning, June 2, 2014  
Tennessee Ballroom B

\* Invited paper

SESSION BP1: Poster Session 1: Sources,  
Instrumentation & Software  
Sunday Evening, June 1, 2014  
5:00 PM  
Summit II

## **BP1.01**

**The New Very Small-Angle Neutron Scattering (VSANS) Diffractometer at NIST** John G. Barker, Charles Glinka, James Moyer and Nick Maliszewskyj; Center for Neutron Research, NIST, Gaithersburg, Maryland.

## **BP1.02**

**<sup>3</sup>He Neutron Spin Filters for Wide-Angle Polarization Analysis on the NCNR MACS Instrument** Qiang Ye<sup>1,2,3</sup>, Wangchun Chen<sup>1,2</sup>, Thomas Gentile<sup>1</sup>, Jeffrey Anderson<sup>1</sup>, Colin Broholm<sup>1,4</sup>, Ross Erwin<sup>1</sup>, John Fuller<sup>1</sup>, Aaron Kirchhoff<sup>1</sup>, Jose Rodriguez<sup>1,2</sup> and Shannon Watson<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, Maryland; <sup>2</sup>University of Maryland, College Park, Maryland; <sup>3</sup>ORNL, Oak Ridge, Tennessee; <sup>4</sup>John Hopkins University, Baltimore, Maryland.

## **BP1.03**

**Superconducting Magnetic Wollaston Prism for Neutron Spin Encoding** Fankang Li<sup>1</sup>, Steven Parnell<sup>1</sup>, William Hamilton<sup>2</sup>, Brian Maranville<sup>3</sup>, Tianhao Wang<sup>1</sup>, Robert Semerad<sup>4</sup>, David Baxter<sup>1</sup>, Jay Cremer<sup>5</sup> and Roger Pynn<sup>1,2</sup>; <sup>1</sup>Center for Exploration of Energy and Matter, Indiana University, Bloomington, Indiana; <sup>2</sup>Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Center for Neutron Scattering, National Institute of Standards and Technology, Gaithersburg, Maryland; <sup>4</sup>Ceraco Ceramic Coating GmbH, Ismaning, Germany; <sup>5</sup>Adelphi Technology Inc., Redwood City, California.

## **BP1.04**

**Stilbene Scintillation Crystals for Fast Neutron Detection** Candace Lynch, Sergey Selin, Anthony Inzalaco and Thomas Caughey; Inrad Optics, Northvale, New Jersey.

## **BP1.05**

**New Directions in Total Scattering at the Lujan Center** Katharine Page, Anna Llobet, Graham King, Joan Siewenie and Hsiu-Wen Wang; Lujan Neutron Scattering Center, Los Alamos National Laboratory, Los Alamos, New Mexico.

## **BP1.06**

**QtiKWS: "Instrument-Free" Approach for SANS Data Treatment** Vitaliy Pipich, Juelich Centre for Neutron Science, Forschungszentrum Juelich GmbH, Garching, Germany.

## **BP1.07**

**A Radial Collimator for a Thermal Time-of-Flight Neutron Chopper Spectrometer** Matthew B. Stone<sup>1</sup>, Doug Abernathy<sup>1</sup>, Jennifer Niedziela<sup>2</sup> and Mark Overbay<sup>2</sup>; <sup>1</sup>Quantum Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Instrument and Source Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## **BP1.08**

**A New TOF-SANS Instrument at the Helmholtz-Zentrum Berlin** Karsten Vogt<sup>1</sup>, Miriam Siebenbuerger<sup>2</sup>, Daniel Clemens<sup>2</sup>, Christian Rabec<sup>2</sup>, Peter Lindner<sup>3</sup>, Margarita Russina<sup>2</sup>, Michael Fromme<sup>2</sup>, Ferenc Mezei<sup>4</sup> and Matthias Ballauff<sup>2,5</sup>; <sup>1</sup>University of Cincinnati, Cincinnati, Ohio; <sup>2</sup>Helmholtz-Zentrum Berlin, Berlin, Germany; <sup>3</sup>Institut Laue-Langevin, Grenoble, France; <sup>4</sup>European Spallation Source, Lund, Sweden; <sup>5</sup>Humboldt University Berlin, Berlin, Germany.

## **BP1.09**

**Calibration of Neutron Powder Diffractometers at SNS** Wenduo Zhou, Peter F. Peterson and Vickie E. Lynch; Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## **10:15 AM \*B1.01**

**Energy-Dependent Neutron Detector Development for a Polychromatic Beam Reflectometer** Charles F. Majkrzak<sup>1</sup>, N. C. Maliszewskyj<sup>1</sup>, A. Osovizky<sup>1,2</sup>, Y. Yehuda-Zada<sup>3,4</sup>, J. Ziegler<sup>1</sup>, K. Pritchard<sup>1</sup>, N. Hadad<sup>1</sup>, J. Cook<sup>1</sup>, E. Binkley<sup>1</sup> and P. Tsai<sup>1</sup>; <sup>1</sup>Center for Neutron Research, NIST, Gaithersburg, Maryland; <sup>2</sup>Rotem Industries Ltd., Rotem Industrial Park, Israel; <sup>3</sup>Ben Gurion University of the Negev, Beer Sheva, Israel; <sup>4</sup>Electronics & Control Laboratories, Nuclear Research Center- Negev, Beer-Sheva, Israel.

## **10:45 AM B1.02**

**The Long and Short Pulse Second SNS Target Stations and Instrument-Moderator Matching** Jinkui Zhao, Lee Robertson, Kenneth Herwig, Franz Gallmeier and Bernie Riemer; ISD, ORNL, Oak Ridge, Tennessee.

## **11:00 AM B1.03**

**KWS-3: Highest Resolution Focusing SANS Diffractometer** Vitaliy Pipich<sup>1</sup>, Zhendong Fu<sup>1</sup>, Alexander Ioffe<sup>1</sup>, Thomas Brueckel<sup>1,2</sup> and Dieter Richter<sup>1,3</sup>; <sup>1</sup>Juelich Centre for Neutron Science, Outstation at MLZ, Forschungszentrum Juelich GmbH, Garching, Germany; <sup>2</sup>Peter Grunberg Institute and Juelich Centre for Neutron Science JCNS-2, Forschungszentrum Juelich GmbH, Juelich, Germany; <sup>3</sup>Institute for Complex Systems and Juelich Centre for Neutron Science JCNS-1, Forschungszentrum Juelich GmbH, Juelich, Germany.

## **11:15 AM B1.04**

**Exploring Microstructures of Materials Using the KOOKABURRA Ultra-Small-Angle Neutron Scattering Instrument at ANSTO** Christine Rehm, ANSTO, Lucas Heights, New South Wales, Australia.

## **11:30 AM B1.05**

**The EQ-SANS Instrument at the Spallation Neutron Source** William T. Heller<sup>1</sup>, Changwoo Do<sup>1</sup>, Christopher B. Stanley<sup>1</sup> and Carrie Y. Gao<sup>2</sup>; <sup>1</sup>Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Instrument and Source Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## **11:45 AM B1.06**

**Understanding Inelastically Scattered Neutrons from Water on a Time-of-Flight Small-Angle Neutron Scattering (SANS) Instrument** Changwoo Do<sup>1</sup>, William T. Heller<sup>1</sup>, Christopher Stanley<sup>1</sup>, Franz X. Gallmeier<sup>2</sup>, Mathieu Doucet<sup>3</sup> and Gregory S. Smith<sup>1</sup>; <sup>1</sup>Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Instrument & Source Design Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Neutron Data analysis & Visualization Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## **12:00 PM B1.07**

**New Methods to Correct the Resolution Errors in Small Angle Neutron Scattering** Xin Li<sup>1</sup>, Wei-Ren Chen<sup>1</sup>, Changwoo Do<sup>1</sup>, Gregory Smith<sup>1</sup>, Lionel Porcar<sup>2</sup>, Yun Liu<sup>4,3</sup>, William A. Hamilton<sup>1</sup>, Takeshi Egami<sup>5</sup> and Luis E. Sanchez-Diaz<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Institut Laue-Langevin, Grenoble, France; <sup>3</sup>NIST Center for Neutron Research, Gaithersburg, Maryland; <sup>4</sup>University of Delaware, Newark, Delaware; <sup>5</sup>The University of Tennessee, Knoxville, Tennessee.

SESSION B2: Sources  
Session Chair: Anna Llobet Megias  
Monday Afternoon, June 2, 2014  
Tennessee Ballroom B

## **1:45 PM \*B2.01**

**Concepts for a Second Spallation Neutron Source Target Station** Kenneth Herwig, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## **2:15 PM B2.02**

**New Concept for Enhanced Flux Neutron Moderator Design** Ferenc Mezei<sup>1,3</sup>, Konstantin Batkov<sup>1</sup>, John Haines<sup>1</sup>, Esben Klinkby<sup>1,2</sup>, Eric Pitcher<sup>1</sup>, Troels Schonfeldt<sup>1,2</sup>, Alan Takibayev<sup>1</sup> and Luca Zanini<sup>1</sup>; <sup>1</sup>Machine Directorate, ESS AB, Lund, Sweden; <sup>2</sup>DTU Nutech, Technical University of Denmark, Risoe, Denmark; <sup>3</sup>Wigner RCF, Hungarian Academy of Sciences, Budapest, Hungary.

### 2:30 PM B2.03

**Introduction of the Reactor Source Spectrometers in China Academy of Engineering Physics and the Recent Research Progress Performed on Them** Jian Gong, Guangai Sun and Bo Chen; Neutron Scattering Laboratory, Institute of Nuclear Physics and Chemistry, China Academy of Engineering Physics, Mianyang, China.

### 2:45 PM B2.05

**Measurement of the Scattering Cross Section for Cold Neutrons on Liquid Parahydrogen** Kyle Grammer, University of Tennessee, Frederick, Maryland.

### 3:00 PM B2.06

**Measurements of Neutron Beam Performance at the Spallation Neutron Source** E. B. Iverson, F. X. Gallmeier, W. Lu, T. C. McClanahan and M. B. Smith; Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

### 3:15 PM B2.07

**SNS Second Target Station Moderator Studies** Franz X. Gallmeier, Wei Lu, Erik B. Iverson, Bernie Riemer, Jinkui Zhao, Ken W. Herwig and Lee Robertson; Instrument and Source Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

### 3:30 PM BREAK

SESSION BP2: Poster Session II: Sources,  
Instrumentation & Software  
Monday Evening, June 2, 2014  
5:30 PM  
Summit II

### BP2.01

**Novel Non-Adiabatic Spin Flipper and Spherical Neutron Polarimeter Using High Tc YBCO Films** Tianhao Wang<sup>1</sup>, Steven Parnell<sup>1</sup>, Fankang Li<sup>1</sup>, William Hamilton<sup>2</sup>, Helmut Kaiser<sup>3</sup>, David Baxter<sup>1</sup> and Roger Pynn<sup>1,2</sup>; <sup>1</sup>Center for the Exploration of Energy and Matter, Indiana University, Bloomington, Indiana; <sup>2</sup>Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>University of Missouri Research Reactor Center, University of Missouri, Columbia, Missouri.

### BP2.02

**CCP-SAS: A Collaborative Computational Project for Small Angle Scattering Modeling** Paul Butler<sup>2,1</sup> and Joseph Curtis<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, Maryland; <sup>2</sup>Chemistry, The University of Tennessee, Knoxville, Tennessee.

### BP2.03

**Wide Field Neutron Imaging System** Michael Fleenor, Lee Robertson and Lowell Crow; NSCD, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

### BP2.04

**Modeling the Phonon Dynamical Structure Factor S(Q,E) from First-Principles Calculations: Recent Progress with CAMM at SNS** Jiawang Hong<sup>1</sup>, Jennifer Niedziela<sup>2</sup>, Chen Li<sup>1</sup>, Vickie Lynch<sup>3</sup> and Olivier Delaire<sup>1</sup>; <sup>1</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Instrument and Source Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Computational Sciences and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

### BP2.05

**Time Dependent SANS Sample Environments Capabilities at NIST** Jeffery Krzywon and Cedric Gagnon; NIST, Gaithersburg, Maryland.

### BP2.06

**An Optimization Framework for Simulations of Experimental Data** Vickie E. Lynch<sup>1</sup>, Jose Borreguero Calvo<sup>1</sup>, Stuart Campbell<sup>1</sup>, Mathieu Doucet<sup>1</sup>, Mark Hagen<sup>2</sup>, Thomas Proffen<sup>1</sup>, Shelly Ren<sup>1</sup> and Andrei Savici<sup>1</sup>; <sup>1</sup>Neutron Data Analysis & Visualization, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Data Management and Software Centre, European Spallation Source, Copenhagen, Denmark.

### BP2.07

**A Real-Time Neutron/Gamma Discrimination Algorithm for a Low Cost LiF:ZnS(Ag) Neutron Detector** Kevin Pritchard<sup>1</sup>, Alon Osovitzky<sup>1,2</sup>, Nicholas Maliszewskyj<sup>1</sup>, Jeffrey Ziegler<sup>1</sup> and Charles Majkrzak<sup>1</sup>; <sup>1</sup>NIST Center for Neutron Research, Gaithersburg, Maryland; <sup>2</sup>Rotem Industries Ltd, Rotem Industrial Park, Israel.

### BP2.08

**McStas Simulation on V-Channel Supermirror Polarizer** Xin T. Tong<sup>1</sup>, Roger Pynn<sup>2</sup> and Lee Robertson<sup>1</sup>; <sup>1</sup>Oak Ridge National Lab, Oak Ridge, Tennessee; <sup>2</sup>Indiana University, Bloomington, Indiana.

### BP2.09

**Neutron Detector Optimization using GEANT 4 Simulation Software** Yaacov Yehuda-Zada<sup>1,2</sup>, Itzhak Orion<sup>2</sup>, Nicholas C. Maliszewskyj<sup>3</sup>, Alon Osovitzky<sup>3,4</sup>; <sup>1</sup>BGU, Beer Sheva, Israel; <sup>2</sup>NRCN, Beer-Sheva, Israel; <sup>3</sup>NIST, Gaithersburg, Maryland; <sup>4</sup>Rotem Industries Ltd, Rotem Industrial Park, Israel.

SESSION BP3: Poster Session III: Sources,  
Instrumentation & Software  
Tuesday Afternoon, June 3, 2014  
3:30 PM  
Summit II

### BP3.01

**Performance of New Double “V” Polarizer and RF Flipper on NG7-SANS at NIST** John G. Barker, Cedric Gagnon, Charles Glinka, Wangchun Chen, Shannon Watson and Kathryn Krycka; NIST, Gaithersburg, Maryland.

### BP3.02

**Obtaining Material Responses Accurately and Efficiently from Time-Resolved Dynamic Flow Neutron Scattering Experiments** Michelle Calabrese, Simon Rogers and Norman J. Wagner; Chemical and Biomolecular Engineering, University of Delaware, Newark, Delaware.

### BP3.03

**Monte Carlo Simulation of the Resolution Ellipsoid for the SEQUOIA Spectrometer** G. E. Granroth<sup>1</sup> and S. E. Hahn<sup>2</sup>; <sup>1</sup>Neutron Data Analysis and Visualization Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

### BP3.04

**SNS Beam Line Control System Update** Kay U. Kasemir, Steven Hartman, Matthew Pearson, Harley Skorpenske and John Sinclair; SNS, Oak Ridge, Tennessee.

### BP3.05

**Lujan Neutron Scattering Center at Los Alamos National Laboratory** Anna Llobet Megias, Lujan Neutron Scattering Center, Los Alamos National Laboratory, Los Alamos, New Mexico.

### BP3.06

**VATES: Software for Advanced Visualization and Quantification of Neutron Scattering Data** Michael Reuter<sup>1</sup>, Toby Perring<sup>2</sup>, Owen Arnold<sup>3</sup>, Alex Buts<sup>2</sup>, Martyn Gigg<sup>3</sup>, Janik Zikovsky<sup>1</sup> and Nick Draper<sup>3</sup>; <sup>1</sup>Neutron Data Analysis and Visualization Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>STFC, Rutherford Appleton Laboratory, Oxfordshire, United Kingdom; <sup>3</sup>Tessella plc, Abingdon, Oxfordshire, United Kingdom.

### BP3.07

**New Methods for Improving Neutron-Gamma Discrimination of Anger Cameras** Cai-Lin Wang and Richard A. Riedel; Oak Ridge National Lab., Oak Ridge, Tennessee.

### BP3.08

**Developments in DISCUS, A Program for Diffuse Scattering and Defect Structure Simulations** Ross Whitfield, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

### BP3.09

**HySpec: New Spectrometer is Hosting Users and Preparing for Polarization Analysis** Barry Winn<sup>1</sup>, Uwe Filges<sup>2</sup>, V. O.

Garlea<sup>1</sup>, Melissa Graves-Brook<sup>3</sup>, Mark Hagen<sup>4,5</sup>, Peter Jiang<sup>3</sup>, Michel Kenzelmann<sup>2</sup>, Larry Passell<sup>6</sup>, Stephen M. Shapiro<sup>6</sup>, Xin Tong<sup>3</sup> and Igor Zaliznyak<sup>6</sup>; <sup>1</sup>Quantum Condensed Matter Division, ORNL, Oak Ridge, Tennessee; <sup>2</sup>Laboratory for Developments & Methods, Paul Scherrer Institut, Villigen PSI, Switzerland; <sup>3</sup>Instrument and Source Division, ORNL, Oak Ridge, Tennessee; <sup>4</sup>Neutron Data Analysis & Visualization, ORNL, Oak Ridge, Tennessee; <sup>5</sup>Data Management and Software, European Spallation Source, Copenhagen, Denmark; <sup>6</sup>Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, Upton, New York.



### BP3.10

#### **Design Constraints and Optimization of a 6LiF:ZnS(Ag) based Neutron Detector** Alon Osovitzky<sup>1,2</sup> Kevin Pritchard<sup>1</sup>,

Jeffrey B. Ziegler<sup>1</sup>, Yaacov Yehuda-Zada<sup>3,4</sup> Nicholas C. Maliszewskyj<sup>1</sup>, Charles F. Majkrzak<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, Maryland; <sup>2</sup>Rotem Industries, Rotem Industrial Park, Israel; <sup>3</sup>NRCN, Beer Sheva, Israel; <sup>4</sup>BGU, Beer Sheva, Israel.

### BP3.11

#### **Computational Science and Education Services** Dwayne John

and Scott Gibson, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

SESSION B3: Software  
Session Chair: Katharine Page  
Wednesday Morning, June 4, 2014  
Tennessee Ballroom B

#### 10:15 AM \*B3.01

##### **Magnetic Pair Distribution Function Analysis: Introduction and Applications** Benjamin Frandsen<sup>1</sup> and Simon J. Billinge<sup>2,3</sup>;

<sup>1</sup>Department of Physics, Columbia University, New York, New York; <sup>2</sup>Department of Applied Physics and Applied Mathematics, Columbia University, New York, New York; <sup>3</sup>Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York.

#### 10:45 AM B3.02

##### **Towards a User-Friendly Software Package for Calculating Spin Wave Excitations** Steven E. Hahn<sup>1</sup>, Randy S. Fishman<sup>2</sup> and Georg Ehlers<sup>1</sup>; <sup>1</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### 11:00 AM B3.03

##### **Monte Carlo Virtual Experiments for Direct Geometry Inelastic Instruments at SNS** Jiao Y. Lin<sup>1</sup>, Hillary Smith<sup>1</sup>, Garrett E. Granroth<sup>2</sup>, Douglas L. Abernathy<sup>2</sup>, Barry L. Winn<sup>2</sup> and Brent Fultz<sup>1</sup>; <sup>1</sup>California Institute of Technology, Pasadena, California; <sup>2</sup>Oak Ridge National Lab, Oak Ridge, Tennessee.

#### 11:15 AM B3.04

##### **Novel Approach to Multi-Orientation Neutron Scattering Data Visualization** Andrei Savici<sup>1</sup>, Michael Reuter<sup>1</sup> and Owen Arnold<sup>2</sup>; <sup>1</sup>ORNL, Oak Ridge, Tennessee; <sup>2</sup>ISIS, Didcot, United Kingdom.

#### 11:30 AM B3.05

##### **MaxEnt: A Length Scale Bridge for Multiscale Nanomaterials** Daniel Olds<sup>1</sup>, Hsiu-Wen Wang<sup>1</sup>, Rex Hjelm<sup>1</sup>, Katharine Page<sup>1</sup> and Devinder Sivia<sup>2</sup>; <sup>1</sup>Los Alamos National Lab, Los Alamos, New Mexico; <sup>2</sup>St. John's College, Oxford, United Kingdom.

#### 11:45 AM B3.06

##### **Workflow Management and Instrument Web Monitoring at the SNS** Mathieu Doucet, ORNL, Oak Ridge, Tennessee.

#### 12:00 PM B3.07

##### **Neutron Spin Echo Data Reduction with DrSPINE** Piotr Zolnierczuk<sup>1</sup>, Olaf Holderer<sup>2</sup>, Michael Monkenbusch<sup>3</sup> and Michael Ohl<sup>1</sup>; <sup>1</sup>Juelich Centre for Neutron Science Outstation at SNS, Forschungszentrum Juelich GmbH, Oak Ridge, Tennessee; <sup>2</sup>Juelich Centre for Neutron Science Outstation at MLZ, Forschungszentrum Juelich GmbH, Garching, Germany; <sup>3</sup>Juelich Centre for Neutron Science and Institute for Complex Systems, Forschungszentrum Juelich GmbH, Juelich, Germany.

SESSION B4: Neutron Optics and Sample Environment  
Session Chair: Ken Herwig  
Wednesday Afternoon, June 4, 2014  
Tennessee Ballroom B

#### 1:45 PM \*B4.01

##### **Neutron Microscope and Focusing SANS Using Axisymmetric Mirrors: Demonstrations and Opportunities** Boris Khaykovich<sup>1</sup>,

Mikhail V. Gubarev<sup>2</sup>, Dazhi Liu<sup>1</sup>, Daniel S. Hussey<sup>3</sup>, David L. Jacobson<sup>3</sup>, Suzanne E. Romaine<sup>4</sup>, Artur Glavic<sup>5</sup>, Valeria Lauter<sup>5</sup>, Lee Robertson<sup>6</sup>, Muhammad Arif<sup>3</sup>, Brian D. Ramsey<sup>2</sup> and David E. Moncton<sup>1</sup>; <sup>1</sup>Nuclear Reactor Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts; <sup>2</sup>Marshall Space Flight Center, NASA, Huntsville, Alabama; <sup>3</sup>Physical Measurement Laboratory, National Institute of Standards and Technology,

Gaithersburg, Maryland; <sup>4</sup>Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts; <sup>5</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>6</sup>Instrument and Source Design Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### 2:15 PM B4.02

##### **Cold Neutron Scattering by Coherent Surface Phonon States**

William A. Hamilton<sup>1,3</sup>, Alberto Cimmino<sup>2</sup>, Andrew Nelson<sup>3</sup> and Mark Lesha<sup>3</sup>; <sup>1</sup>Neutron Instrument & Source Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>School of Physics, University of Melbourne, Melbourne, Victoria, Australia; <sup>3</sup>Bragg Institute, Australian Nuclear Science and Technology Organisation, Lucas Heights, New South Wales, Australia.

#### 2:30 PM B4.03

##### **Development of 25 - 30 T Magnets for Neutron Scattering at the NHFML** Mark Bird, NHMFL - FSU, Tallahassee, Florida.

#### 2:45 PM B4.04

##### **Status of Sample Environment at SNS and HFIR**

Hans-Jochen Lauter, ORNL, Oak Ridge, Tennessee.

#### 3:00 PM B4.05

##### **Minimizing Pressure In-Homogeneities for Large Samples in High Pressure Neutron Scattering Measurements**

Juscelino B. Leao, NCNR, NIST, Gaithersburg, Maryland.

#### 3:15 PM B4.06

##### **High-Temperature Sample Environment Template for Experiment Simulations on DGS Instruments at the SNS** Hillary Smith<sup>1</sup>, Jiao Lin<sup>1</sup>, Garrett Granroth<sup>2</sup>, Doug Abernathy<sup>3</sup> and Brent Fultz<sup>1</sup>; <sup>1</sup>California Institute of Technology, Pasadena, California; <sup>2</sup>Neutron Data Analysis and Visualization Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### 3:30 PM BREAK

SESSION B5: Instrumentation II  
Session Chairs: Richard Ibberson and Dan Neumann  
Wednesday Afternoon, June 4, 2014  
Tennessee Ballroom B

#### 4:00 PM B5.01

##### **IMAGINE, A Quasi-Laue Single Crystal Neutron Diffractometer At The HFIR** Flora Meilleur, ORNL / NCSU, Oak Ridge, Tennessee.

#### 4:15 PM B5.02

##### **The Vision Spectrometer at the Spallation Neutron Source**

Christoph U. Wildgruber<sup>1</sup>, Malcolm J. Cochran<sup>2</sup>, Lacy L. Jones<sup>1</sup>, Yongqiang Chen<sup>1</sup> and Anibal J. Ramirez-Cuesta<sup>1</sup>; <sup>1</sup>NCSU, ORNL, Oak Ridge, TN, Tennessee; <sup>2</sup>JCNS, Forschungszentrum, Juelich, Juelich, Germany.

#### 4:30 PM B5.03

##### **Towards a Neutron Microscope at NIST** Daniel Hussey<sup>1</sup>, David

Jacobson<sup>1</sup>, Dazhi Liu<sup>2</sup>, Boris Khaykovich<sup>2</sup> and Mikhail Gubarev<sup>3</sup>; <sup>1</sup>NIST, Gaithersburg, Maryland; <sup>2</sup>MIT, Cambridge, Massachusetts; <sup>3</sup>NASA, Huntsville, Alabama.

#### 4:45 PM B5.04

##### **SIKA - The Cold Triple Axis Spectrometer at ANSTO**

Jason S. Gardner, Neutron Group, NSRRC, Hsinchu, Taiwan.

#### 5:00 PM B5.05

##### **The Progress of Neutron Diffraction Stress Analysis**

**Technique at China Academy of Engineering Physics** Guangai Sun, Bo Chen, Hong Wang and Jian Li; Neutron Scattering Laboratory, Institute of Nuclear Physics and Chemistry, China Academy of Engineering Physics, Mianyang, China.

#### 5:15 PM B5.06

##### **CORELLI: The Elastic Diffuse Scattering Spectrometer at SNS**

Feng Ye<sup>1</sup>, Ross E. Whitfield<sup>3</sup>, Mark Hagen<sup>3</sup>, Stephan Rosenkranz<sup>2</sup> and Ray Osborn<sup>2</sup>; <sup>1</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Knoxville, Tennessee; <sup>2</sup>Materials Science Division, Argonne National Laboratory, Argonne, Illinois; <sup>3</sup>Neutron Data Analysis and Visualization Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### **BP4.01**

**Temperature Dependence of Background Scattering from Materials Found in SANS** John G. Barker and David Mildner; NIST, Gaithersburg, Maryland.

#### **BP4.02**

**In Situ Experiment Scan Optimization Using an EPICS-Based Control System on the VULCAN Engineering Materials Diffractometer at the SNS** Matthew Frost, Harley Skorpenske, Kay Kasemir, Matthew Pearson and Steven Hartman; Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### **BP4.03**

**Understanding Geometric Distortion of the Tube Detectors on SANS Instruments at ORNL** Lilin He, Changwoo Do, Shuo Qian, George D. Wignall, William T. Heller, Kenneth C. Kenneth and Gregory S. Smith; Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### **BP4.04**

**Integration of Neutron Time-of-Flight Single-Crystal Bragg Peaks in Reciprocal Space** Mads R. Joergensen<sup>1</sup>, Arthur J. Schultz<sup>2</sup>, Xiaoping Wang<sup>3</sup>, Ruth L. Mikkelsen<sup>4</sup>, Dennis J. Mikkelsen<sup>1</sup>, Vickie E. Lynch<sup>5</sup>, Peter F. Peterson<sup>5</sup>, Mark L. Green<sup>6</sup> and Christina M. Hoffmann<sup>3</sup>; <sup>1</sup>Center for Materials Crystallography, Dept. of Chemistry & iNano, Aarhus University, Aarhus, Denmark; <sup>2</sup>X-Ray Science Division, Argonne National Laboratory, Argonne, Illinois; <sup>3</sup>Chemical and Engineering Materials Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Department of Mathematics, Statistics and Computer Science, University of Wisconsin-Stout, Menomonie, Wisconsin; <sup>5</sup>Neutron Data Analysis and Visualization Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>6</sup>Tech-X Corporation, Tech-X Corporation, New York.

#### **BP4.05**

**Optimization of Axisymmetric Grazing-Incidence Focusing Optics Utilized in Neutron Imaging** Dazhi Liu<sup>1</sup>, Mikhail V. Gubarev<sup>2</sup>, Daniel S. Hussey<sup>3</sup>, David L. Jacobson<sup>3</sup>, David E. Moncton<sup>1,4</sup> and Boris Khaykovich<sup>1</sup>; <sup>1</sup>Nuclear Reactor Laboratory, MIT, Cambridge, Massachusetts; <sup>2</sup>Marshall Space Flight Center, NASA, Huntsville, Alabama; <sup>3</sup>Physical Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, Maryland; <sup>4</sup>Department of Physics, MIT, Cambridge, Massachusetts.

#### **BP4.06**

**Continuous Source, Polychromatic Beam Powder Neutron Diffractometer** Charles F. Majkrzak, Jason M. Simmons, Jeremy C. Cook, Richard M. Ibberson and Dan A. Neumann; Center for Neutron Research, NIST, Gaithersburg, Maryland.

#### **BP4.07**

**Mantid Data Reduction and Visualization at SNS and HFIR** Jean-C. Bilheux, Jose M. Borreguerro-Calvo, Stuart I. Campbell, Mathieu Doucet, Vickie E. Lynch, Dennis J. Mikkelsen, Ruth L. Mikkelsen, Peter F. Peterson, Shelly Ren, Michael A. Reuter, Andrei T. Savici, Russell J. Taylor, Ross E. Whitfield, Wenduo Zhou and Janik Zikovsky; Neutron Scattering Science Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### **BP4.08**

**Wavelength and Bandwidth Tunable Diode Laser System for SEOP** Aleksandr Rysanyanskiy<sup>1</sup>, Jeremy Lawrence<sup>1</sup>, Lawrence Chase<sup>1</sup>, Vadim Smirnov<sup>1</sup>, Oleksiy Mokhun<sup>1</sup>, Alexei Glebov<sup>1</sup> and Leonid Glebov<sup>2</sup>; <sup>1</sup>OptiGrate Inc., Oviedo, Florida; <sup>2</sup>CREOL / The College of Optics and Photonics, University of Central Florida, Orlando, Florida.

#### **BP4.09**

**A Comparison of the Four Chopper Spectrometers at the Spallation Neutron Source** Matthew B. Stone<sup>1</sup>, Jennifer Niedziela<sup>2</sup>, Douglas Abernathy<sup>1</sup>, Lisa DeBeer-Schmitt<sup>2</sup>, Ovidiu Garlea<sup>1</sup>, Garrett Granroth<sup>1</sup>, Georg Ehlers<sup>1</sup>, Sasha Kolesnikov<sup>3</sup>, Andrey Podlesnyak<sup>1</sup>, Barry Winn<sup>1</sup> and Melissa Graves-Brook<sup>2</sup>; <sup>1</sup>Quantum Condensed Matter Science Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Instrument and Source Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Chemical & Engineering Materials Div, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### **BP4.10**

**Progress of Data Acquisition for High Neutron Flux Instruments at the Spallation Neutron Source** Bogdan Vacaliuc<sup>1</sup>, Klemen Vodopivec<sup>2</sup>, Marie X. Yao<sup>1</sup> and James A. Kohl<sup>1</sup>; <sup>1</sup>Spallation Neutron Source (SNS), Oak Ridge National Laboratory (ORNL), Oak Ridge, Tennessee; <sup>2</sup>Cosylab, Ljubljana, Slovenia.

SESSION B6: Spin Polarizers  
Session Chair: Charles Majkrzak  
Thursday Morning, June 5, 2014  
Tennessee Ballroom B

#### **9:45 AM \*B6.01**

**New Technologies for Spin Manipulation Using High Temperature Superconductors** Steven R. Parnell, CEEM - Center for the Exploration of Energy and Matter, Indiana University, Bloomington, Indiana.

#### **10:15 AM B6.02**

**In Situ Neutron Reflectometry During Thin Film Growth by Sputter Deposition** Wolfgang Kreuzpaintner<sup>1</sup>, Birgit Wiedemann<sup>1</sup>, Sina Mayr<sup>1</sup>, Amitesh Paul<sup>1</sup>, Thomas Mairoser<sup>2</sup>, Andreas Schmehl<sup>2</sup>, Alexander Herrnberger<sup>2</sup>, Jochen Stahn<sup>5</sup>, Jean-Francois Moulin<sup>4</sup>, Korelis Panagiotis<sup>5</sup>, Martin Haese-Seiler<sup>4</sup>, Matthias Pomm<sup>4</sup>, Peter Böni<sup>1</sup> and Jochen Mannhart<sup>3</sup>; <sup>1</sup>Physik-Department E21, Technische Universität München, Garching, Germany; <sup>2</sup>Zentrum fuer Elektronische Korrelationen und Magnetismus, Lehrstuhl fuer Experimentalphysik VI, Universität Augsburg, Augsburg, Germany; <sup>3</sup>Max-Planck-Institut fuer Festkörperforschung, Stuttgart, Germany; <sup>4</sup>Helmholtz-Zentrum Geesthacht Zentrum für Material- und Küstenforschung GmbH, Geesthacht, Germany; <sup>5</sup>Laboratory for Neutron Scattering, Paul Scherrer Institut, Villigen PSI, Switzerland.

#### **10:30 AM B6.03**

**High Performance Polarized Thermal Triple-Axis Spectrometer** Wangchun Chen<sup>1,2</sup>, Ross Erwin<sup>2</sup>, Shannon Watson<sup>2</sup>, Thomas Gentile<sup>2</sup> and Jeffrey Lynn<sup>2</sup>; <sup>1</sup>University of Maryland, College Park, Maryland; <sup>2</sup>NIST, Gaithersburg, Maryland.

#### **10:45 AM B6.04**

**Development of In Situ Polarized <sup>3</sup>He Neutron Spin Filters at Oak Ridge National Laboratory** Chenyang Jiang, Xin Tong, Benjamin Kadron, Dan Brown and Lee Robertson; Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### **11:00 AM B6.05**

**Continuously Operating <sup>3</sup>He as a Neutron Spin Filter for Spin Echo Scattering Angle Measurement (SESAME)** Ke Li<sup>1</sup>, Haiyang Yan<sup>1</sup>, Steven Parnell<sup>1</sup>, Roger Pynn<sup>1,2</sup> and William M. Snow<sup>1</sup>; <sup>1</sup>Center for Exploration of Energy and Matter, Indiana University, Bloomington, Indiana; <sup>2</sup>Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

# C: Hard Condensed Matter

\* Invited paper

SESSION CP1: Poster Session: Hard Condensed Matter  
Sunday Evening, June 1, 2014  
5:00 PM  
Summit II

## CP1.01

**Local and Global Orbital Ordered State in  $\text{La}_{1-x}\text{Y}_x\text{VO}_3$**   
Shin-ichiro Yano<sup>1</sup>, Despina Louca<sup>1</sup>, Jiaqiang Yan<sup>2</sup>, Jörg Neufeind<sup>3</sup>, Jianshi Zhou<sup>4</sup> and John B Goodenough<sup>4</sup>; <sup>1</sup>Physics, Univ. of Virginia, Charlottesville, Virginia; <sup>2</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Chemical and Engineering Materials Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Materials Science and Engineering Program/Mechanical Engineering, Univ. of Texas, Austin, Texas.

## CP1.02

**Impact of Oxygen Vacancy Profiles on the Magnetic Properties of  $\text{La}_{0.80}\text{Sr}_{0.20}\text{CoO}_3$**  Michael D. Biegalski<sup>1</sup>, Liang Qiao<sup>1</sup>, Alex Belianinov<sup>1</sup>, Sergei V. Kalinin<sup>1</sup>, Haile Ambaye<sup>2</sup> and Valeria Lauter<sup>2</sup>; <sup>1</sup>Center for Nanophase Materials Science, Oak Ridge National Lab, Oak Ridge, Tennessee; <sup>2</sup>Neutron Scattering Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## CP1.03

**Magnetic Studies of 5d Materials Containing Novel Insulating States with Neutron Scattering** Stuart Calder<sup>1</sup>, Guixin Cao<sup>1,2</sup>, Satoshi Okamoto<sup>1</sup>, Jong-Woo Kim<sup>3</sup>, Valentino Cooper<sup>1</sup>, Brian Sales<sup>1</sup>, Mark Lumsden<sup>1</sup>, David Mandrus<sup>2,1</sup> and Andrew Christianson<sup>1</sup>; <sup>1</sup>ORNL, Knoxville, Tennessee; <sup>2</sup>University of Tennessee, Knoxville, Tennessee; <sup>3</sup>Advanced Photon Source, Argonne, Illinois.

## CP1.04

**Collective Magnetic Dynamics in  $\text{Ni}_3\text{V}_2\text{O}_8$**  Georg Ehlers<sup>1</sup>, Steven Hahn<sup>1</sup>, Andrey Podlesnyak<sup>1</sup>, Randy Fishman<sup>2</sup>, Oksana Zaharko<sup>3</sup>, Matthias Frontzek<sup>3</sup> and Michel Kenzelmann<sup>4</sup>; <sup>1</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Laboratory for Neutron Scattering, Paul-Scherrer Institute, Villigen, Switzerland; <sup>4</sup>Laboratory for Developments and Methods, Paul-Scherrer Institute, Villigen, Switzerland.

## CP1.05

**Magnetic Structure of the Self Doping Terbium Orthomanganite** Hao Zhang<sup>1</sup>, Roxana Flacau<sup>2</sup>, Junliang Sun<sup>1</sup>, Guobao Li<sup>1</sup>, Fuhui Liao<sup>1</sup> and Jianhua Lin<sup>1</sup>; <sup>1</sup>Peking University, Beijing, China; <sup>2</sup>Chalk River Laboratories, Canadian Neutron Beam Centre, Chalk River, Ontario, Canada.

## CP1.06

**Pressure-Induced Structural Phase Transition in  $\text{CeNi}$**  Alexey Mirmelstein<sup>1</sup>, Vladimir N. Matvienko<sup>1</sup>, Oleg V. Kerbel<sup>1</sup>, Andrey Podlesnyak<sup>2</sup>, Alexander I. Kolesnikov<sup>3</sup>, António F. Dos Santos<sup>2</sup>, Bayrammurad I. Saparov<sup>4</sup>, Athena S. Sefat<sup>4</sup> and James G. Tobin<sup>5</sup>; <sup>1</sup>Department of Experimental Physics, RFNC-VNIITF, Snezhinsk, Chelyabinsk Region, Russian Federation; <sup>2</sup>Quantum Condensed Matter Div, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Chemical and Engineering Materials Div., Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Materials Science and Engineering Div., Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>5</sup>Lawrence Livermore National Laboratory, Livermore, California.

## CP1.07

**Reexamination of Soft Mode Behavior in  $\text{PbTe}$**  Richard H. Roberts<sup>1</sup>, Kirsten M. Jensen<sup>1</sup>, Emil S. Bozin<sup>2</sup>, Simon J. Billinge<sup>1,2</sup> and Stephen M. Shapiro<sup>2</sup>; <sup>1</sup>Materials Science and Engineering, Columbia University, New York, New York; <sup>2</sup>Condensed Matter Physics and Materials Science, Brookhaven National Lab, Upton, New York.

## CP1.08

**Effect of Chemical and Hydrostatic Pressure on In-Plane and Interplane Exchange Interactions in Bi-Layer Manganites** Kirill Shaykhutdinov<sup>1</sup>, Andrey Podlesnyak<sup>2</sup>, Antonio F. Moreira Dos Santos<sup>2</sup>, Zheng Gai<sup>3</sup>, Steven Hahn<sup>2</sup> and Georg Ehlers<sup>2</sup>; <sup>1</sup>Kirensky Institute of Physics, Krasnoyarsk, Russian Federation; <sup>2</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, TN

37831, USA, Oak Ridge, Tennessee; <sup>3</sup>Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, Oak Ridge, Tennessee.

## CP1.09

**Magnetoelectric Coupling in Type-II Multiferroic  $\text{Co}_3\text{TeO}_6$**  Chin-Wei Wang, National Synchrotron Radiation Research Center, Hsinchu, Taiwan.

SESSION C1: Complex Oxide Heterostructures  
Session Chair: Valerie Lauter  
Monday Morning, June 2, 2014  
Summit I

## 10:15 AM \*C1.01

**Emergent Magnetic Phenomena at Complex Oxide Interfaces** Yuri Suzuki, Applied Physics, Stanford University, Stanford, California.

## 10:45 AM C1.02

**Emergent Single State in Magnetic Oxide Superlattices** Artur G. Glavic<sup>1</sup>, Paul Zakalck<sup>2</sup>, Jürgen Schubert<sup>3</sup> and Stefan Mattau<sup>2</sup>; <sup>1</sup>Quantum Condensed Matter Division, Oak Ridge National Lab, Oak Ridge, Tennessee; <sup>2</sup>Juelich Centre for Neutron Science JCNS-2 and Peter Gruenberg Institut PGI-4, Forschungszentrum Juelich GmbH, Juelich, Germany; <sup>3</sup>Peter Gruenberg Institut PGI-9 and JARA-FIT, Forschungszentrum Juelich GmbH, Juelich, Germany.

## 11:00 AM C1.03

**Effects of Interface Engineering on Magnetization Structure in  $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3/\text{SrTiO}_3$  Heterostructures** M. Huijben<sup>1</sup>, Yaohua Liu<sup>2</sup>, H. Boschker<sup>1</sup>, V. Lauter<sup>3</sup>, R. Egoavil<sup>4</sup>, J. Verbeeck<sup>1</sup>, S. G. te Velthuis<sup>2</sup>, G. Rijnders<sup>1</sup> and G. Koster<sup>1</sup>; <sup>1</sup>Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, Enschede, Netherlands; <sup>2</sup>Materials Science Division, Argonne National Laboratory, Lemont, Illinois; <sup>3</sup>Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Electron Microscopy for Materials Science, University of Antwerp, Antwerp, Belgium.

## 11:15 AM \*C1.04

**Probing Complex Oxide Heterostructures via Neutron Study** Xianglin Ke, Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan.

## 11:45 AM C1.05

**The Influence of Strain and Orientation on  $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$  Thin Films: Controlling Interface Magnetism via Oxygen Vacancy Ordering** Shameek Bose<sup>1</sup>, Manish Sharma<sup>1</sup>, Maria Torija<sup>1</sup>, Jaume Gazquez<sup>2,3</sup>, Maria Varela<sup>2,3</sup>, Steve Pennycook<sup>3</sup>, Valeria Lauter<sup>4</sup>, Haile Ambaye<sup>4</sup>, Rick Goyette<sup>4</sup>, Mike Fitzsimmons<sup>5</sup> and Chris Leighton<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, Minnesota; <sup>2</sup>Universidad Complutense de Madrid, Madrid, Spain; <sup>3</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>5</sup>Los Alamos Neutron Science Center, Los Alamos National Laboratory, Los Alamos, New Mexico.

## 12:00 PM C1.06

**Neutron Investigations of Multiferroic  $\text{LuFeO}_3$  Thin Films** William Ratcliff<sup>1</sup>, Julie Borchers<sup>1</sup>, Peter Schiffer<sup>3</sup>, Jarret Moyer<sup>3</sup>, Julia Mundy<sup>2</sup>, Charles Brooks<sup>2</sup>, Hena Das<sup>4</sup>, Craig Fennie<sup>4</sup> and Darrel Schlom<sup>2</sup>; <sup>1</sup>NCNR, NIST, Gaithersburg, Maryland; <sup>2</sup>Materials Science and Engineering, Cornell, Ithaca, New York; <sup>3</sup>Physics, University of Illinois, Urbana-Champaign, Illinois; <sup>4</sup>Applied Physics, Cornell, Ithaca, New York.

SESSION C2: Frustration in Complex Oxides  
Session Chair: Collin Broholm  
Monday Afternoon, June 2, 2014  
Summit I

## 1:45 PM \*C2.01

**Spin Jams, Frustration, and Exotic Entropy Scaling** Israel Klich and Seunghun Lee; Physics, University of Virginia, Charlottesville, Virginia.

## 2:15 PM C2.02

**Contributions from Configurational and Vibrational Entropy in Glassy  $\text{CuZr}$**  Hillary Smith<sup>1</sup>, Chen Li<sup>2</sup>, Marios Demetriou<sup>1</sup>, Matthew Stone<sup>3</sup>, Doug Abernathy<sup>3</sup> and Brent Fultz<sup>1</sup>; <sup>1</sup>California Institute of Technology, Pasadena, California; <sup>2</sup>Materials Science and

Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

### 2:30 PM C2.03

**Structure Transitions in the Low-Dimensional Compounds BaMn<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>** Jie Ma<sup>1</sup>, Clarina R. Dela Cruz<sup>1</sup>, Tao Hong<sup>1</sup>, Wei Tian<sup>1</sup>, Adam Aczel<sup>1</sup>, Songxue Chi<sup>1</sup>, Jiaqiang Yan<sup>2,3</sup>, Zhiling Dun<sup>4</sup>, Haidong Zhou<sup>4</sup> and Masaaki Matsuda<sup>1</sup>; <sup>1</sup>Quantum Condensed Matter Division, OAK RIDGE NATIONAL LABORATORY, Oak Ridge, Tennessee; <sup>2</sup>Materials Science and Technology Division, OAK RIDGE NATIONAL LABORATORY, Oak Ridge, Tennessee; <sup>3</sup>Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee; <sup>4</sup>Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee.

### 2:45 PM C2.04

**Long Range Magnetic Order in Spin-orbit-coupled Double Perovskites Ba<sub>2</sub>YRuO<sub>6</sub> and Ba<sub>2</sub>CaOsO<sub>6</sub> Probed with Neutron Scattering and Muon Spin Relaxation: Comparison with Theory and Disordered Ba<sub>2</sub>YReO<sub>6</sub> and Ba<sub>2</sub>YMoO<sub>6</sub>** Jeremy P. Carlo<sup>1</sup>, J. P. Clancy<sup>2</sup>, C. M. Thompson<sup>3</sup>, Y. J. Uemura<sup>4</sup>, J. E. Greedan<sup>3</sup>, B. D. Gaulin<sup>4</sup>

<sup>1</sup>Villanova University, Villanova, Pennsylvania; <sup>2</sup>University of Toronto, Toronto, Ontario, Canada; <sup>3</sup>McMaster, Hamilton, Ontario, Canada; <sup>4</sup>Columbia University, New York, New York.

### 3:00 PM C2.05

**Orbital Crystallization from a Glassy State in Ba<sub>3</sub>CoSb<sub>2</sub>O<sub>9</sub>** Bing Li<sup>1</sup>, Despina Louca<sup>1</sup>, Mikhail Feyngenson<sup>2</sup>, Joerg Neufeind<sup>2</sup> and Craig Brown<sup>3</sup>; <sup>1</sup>Physics, University of Virginia, Charlottesville, Virginia; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>National Institute of Standards and Technology, Gaithersburg, Maryland.

### 3:15 PM C2.06

**Magnons, Trigonal Fields and Double Orbital Order in the Spinel Compound, FeV<sub>2</sub>O<sub>4</sub>** Gregory J. MacDougall<sup>1</sup>, I. Brodsky<sup>1</sup>, A. A. Aczel<sup>2</sup>, V. O. Garlea<sup>2</sup>, G. E. Granroth<sup>2</sup>, T. Hong<sup>2</sup>, A. D. Christianson<sup>2</sup>, H. D. Zhou<sup>3</sup> and S. E. Nagler<sup>2</sup>; <sup>1</sup>Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois; <sup>2</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Department of Physics, University of Tennessee, Knoxville, Tennessee.

### 3:30 PM BREAK

SESSION C3: Exotic Phase Transitions in Complex Materials I

Session Chair: Igor Zaloznak  
Monday Afternoon, June 2, 2014  
Summit I

### 4:00 PM \*C3.01

**Exploring the Mechanism of the Metal-Insulator Transition of a Carrier Doped Spin-Orbit Mott Insulator** Stephen Wilson, Boston College, Chestnut Hill, Massachusetts.

### 4:30 PM C3.02

**Field-Induced Magnetic Phase Transitions in Ti-Doped Ca<sub>3</sub>Ru<sub>2</sub>O<sub>7</sub> Bilayer Ruthenates** Mengze Zhu<sup>1</sup>, Jin Peng<sup>2</sup>, Karel Prokes<sup>3</sup>, S. Matas<sup>3</sup>, Tao Hong<sup>4</sup>, Zhiqiang Mao<sup>2</sup> and Xianglin Ke<sup>1</sup>; <sup>1</sup>Michigan State University, East Lansing, Michigan; <sup>2</sup>Department of Physics and Engineering Physics, Tulane University, New Orleans, Louisiana; <sup>3</sup>Helmholtz Zentrum Berlin, Berlin, Germany; <sup>4</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee.

### 4:45 PM C3.03

**Time-Resolved Neutron Scattering Study of Magnetic Structural Change in Frustrated Magnets** Kiyochiro Motoya<sup>1</sup>, Masato Hagihara<sup>1</sup> and Masaaki Matsuda<sup>2</sup>; <sup>1</sup>Physics, Tokyo University of Science, Noda, Japan; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee.

### 5:00 PM C3.04

**Phase Transition from An Orbital-Ordered to A Frustration-Relieved Non-Collinear Spin State in Spinel (Mn<sub>1-x</sub>Co<sub>x</sub>)V<sub>2</sub>O<sub>4</sub>** Jun Hee Lee<sup>1</sup>, Steven E. Hahn<sup>2</sup> and Randy S. Fishman<sup>1</sup>; <sup>1</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

### 5:15 PM C3.05

**Structure and Dynamics of CdTe Studied by X-Ray and Neutron Scattering** Jennifer L. Niedziela and Matthew B. Stone; Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

SESSION CP2: Poster Session II: Hard Condensed Matter

Monday Evening, June 2, 2014

5:30 PM

Summit II

### CP2.01

**Crystal Field Excitations in ErVO<sub>3</sub>** Arnab Banerjee<sup>1</sup>, Garrett Granroth<sup>1</sup>, Haidong Zhao<sup>2</sup>, Zhiling Dun<sup>2</sup> and Stephen E. Nagler<sup>1,2</sup>; <sup>1</sup>QCMD, ORNL, Knoxville, Tennessee; <sup>2</sup>Dept. Physics, UT, Knoxville, Tennessee.

### CP2.02

**Neutron Diffraction Study of the Magnetic Phase Diagram of Dysprosium with 1.0 and 1.5 Tesla Field Applied Parallel to the A-Axis** Lowell Crow<sup>1</sup>, Lee Robertson<sup>1</sup>, Jian Yu<sup>2</sup> and Gary Mankey<sup>2</sup>; <sup>1</sup>Instrument and Source Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Physics and Astronomy, University of Alabama, Tuscaloosa, Alabama.

### CP2.03

**Vortices in Interacting Multilayered Nanowires: Theory vs SANS Experiment** Olena Tartakivska<sup>1</sup>, Kathryn Krycka<sup>1</sup>, Alexander Grutter<sup>1</sup>, Julie Borchers<sup>1</sup>, Brian Kirby<sup>1</sup>, Jung Jin Park<sup>2</sup>, Alison Flatau<sup>2</sup> and Bethany Stadler<sup>3</sup>; <sup>1</sup>NIST Center For Neutron Research, Gaithersburg, Maryland; <sup>2</sup>University of Maryland, College Park, Maryland; <sup>3</sup>University of Minnesota, Minneapolis, Minnesota.

### CP2.04

**Exploration of Ice Rule in Nanoengineered Honeycomb Lattice** Harrison Knoll<sup>1</sup>, D. K. Singh<sup>1</sup>, H. Kaiser<sup>2</sup> and K. Krycka<sup>3</sup>; <sup>1</sup>Physics and Astronomy, University of Missouri, Columbia, Missouri; <sup>2</sup>MURR-University of Missouri, Columbia, Missouri; <sup>3</sup>NIST Center for Neutron Research, Gaithersburg, Maryland.

### CP2.05

**Complicated Magnetic Structure in Nd<sub>2-x</sub>Sr<sub>x</sub>NiO<sub>4</sub> (x = 0.7)** Riki Kobayashi<sup>1</sup>, Hideki Yoshizawa<sup>1</sup>, Masaaki Matsuda<sup>2</sup>, Ryoichi Kajimoto<sup>3</sup>, Kyoko Ishizaka<sup>4</sup> and Yoshinori Tokura<sup>5</sup>; <sup>1</sup>Neutron Science Laboratory, Institute for Solid State Physics, Ibaraki, Japan; <sup>2</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Materials and Life Science Division, J-PARC Center, Ibaraki, Japan; <sup>4</sup>Department of Applied Physics, The University of Tokyo, Tokyo, Japan; <sup>5</sup>Center for Emergent Matter Science, RIKEN, Saitama, Japan.

### CP2.06

**The Anharmonic Thermal Stability of Rutile TiO<sub>2</sub>** Tian Lan<sup>1</sup>, Chen W. Li<sup>2</sup> and Brent Fultz<sup>1</sup>; <sup>1</sup>Applied Physics, California Institute of Technology, Pasadena, California; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee.

### CP2.07

**Vertically Controllable Ferromagnetic Phase Boundary in Compositionally Graded NiCu Films** Brian Kirby<sup>1</sup>, Hillary Belliveau<sup>2</sup>, Dustin Belyca<sup>2</sup> and Casey Miller<sup>2</sup>; <sup>1</sup>Center for Neutron Research, NIST, Gaithersburg, Maryland; <sup>2</sup>Physics, University of South Florida, Tampa, Florida.

### CP2.08

**Observation of Dramatically Increased Mass Recoil in a System of Absorbed Supercritical Hydrogen** Raina J. Olsen, Oak Ridge National Laboratory, Knoxville, Tennessee.

### CP2.09

**Studying Nanodomains in Lead-Free Relaxor Ferroelectric CaxBa<sub>1-x</sub>Nb<sub>2</sub>O<sub>6</sub>** Chandra Shekhar Pandey<sup>1</sup>, Manfred Burianek<sup>2</sup>, Manfred Muhlberg<sup>2</sup> and Jürgen Schreuer<sup>1</sup>; <sup>1</sup>Earth Sciences, Ruhr University Bochum, Bochum, NRW, Germany; <sup>2</sup>Crystallography, University of Cologne, Cologne, NRW, Germany.

### CP2.10

**Coexistence of Half-Metallic Itinerant Ferromagnetism with Local-Moment Antiferromagnetism in Ba<sub>0.60</sub>K<sub>0.40</sub>Mn<sub>2</sub>As<sub>2</sub>** Benjamin Ueland<sup>1,2</sup>, Abhishek Pandey<sup>1,2</sup>, S. Yeninas<sup>1,2</sup>, A. Kreyssig<sup>1,2</sup>, A. Sapkota<sup>1,2</sup>, Yang Zhao<sup>3,4</sup>, J. S. Helton<sup>3</sup>, J. W. Lynn<sup>3</sup>, R. J. McQueeney<sup>1,2</sup>, Y. Furukawa<sup>1,2</sup>, A. I. Goldman<sup>1,2</sup> and D. C. Johnston<sup>1,2</sup>; <sup>1</sup>Ames Laboratory, Ames, Iowa; <sup>2</sup>Department of Physics

and Astronomy, Iowa State University, Ames, Iowa; <sup>3</sup>NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland; <sup>4</sup>Department of Materials Science and Engineering, University of Maryland, College Park, Maryland.

SESSION C4: Fe-based Superconductors  
Session Chair: Stephan Wilson  
Tuesday Morning, June 3, 2014  
Summit I

**10:15 AM \*C4.01**

**Neutron Scattering Study on NaFe<sub>1-x</sub>CoxAs** Chenglin Zhang,  
<sup>1</sup>Rice Univ, Physics Dept, Houston, Texas; <sup>2</sup>Physics, UTK, Knoxville, Tennessee.

**10:45 AM C4.02**

**Spin Dynamics in FeAs** Andrey Podlesnyak<sup>1</sup>, Georg Ehlers<sup>1</sup>, Steven Hahn<sup>1</sup>, Krzysztof Gofryk<sup>2</sup> and Athena S. Sefat<sup>2</sup>; <sup>1</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Materials Science and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

**11:00 AM C4.03**

**A Study of the Spin-Density Wave Transformation in BaFe<sub>2</sub>(As<sub>1-x</sub>Px)<sub>2</sub> Using High-Resolution Neutron Diffraction** Jared M. Allred<sup>1</sup>, Keith M. Taddei<sup>1,2</sup>, Dan E. Bugaris<sup>1</sup>, Sevda Avci<sup>3</sup>, Dennis Brown<sup>2</sup>, Duck Young Chung<sup>1</sup>, Helmut Claus<sup>1</sup>, Ashfia Huq<sup>4</sup>, Clarina Dela Cruz<sup>5</sup>, Mercouri Kanatzidis<sup>6</sup>, Stephan Rosenkranz<sup>1</sup>, Omar Chmaissem<sup>1,2</sup> and Raymond Osborn<sup>1</sup>; <sup>1</sup>Materials Science Division, Argonne National Laboratory, Lemont, Illinois; <sup>2</sup>Department of Physics, Northern Illinois University, DeKalb, Illinois; <sup>3</sup>Department of Materials Science and Engineering, Afyon Kocatepe University, Afyon, Turkey; <sup>4</sup>Spallation Neutron Source, Oak Ridge National Lab, Oak Ridge, Tennessee; <sup>5</sup>High Flux Isotope Reactor, Oak Ridge National Lab, Oak Ridge, Tennessee; <sup>6</sup>Department of Chemistry, Northwestern University, Evanston, Illinois.

**11:15 AM C4.04**

**Anisotropic Resonance Peaks in Iron-Based Superconductors Studied by Neutron Scattering** C. H. Lee<sup>1</sup>, P. Steffens<sup>2</sup>, N. Qureshi<sup>3</sup>, K. Kihou<sup>1</sup>, M. Nakajima<sup>1</sup>, A. Iyo<sup>1</sup>, H. Eisaki<sup>1</sup> and M. Braden<sup>3</sup>; <sup>1</sup>AIST, Tsukuba, Ibaraki, Japan; <sup>2</sup>ILL, Grenoble, France; <sup>3</sup>Universitat zu Koln, Koln, Germany.

**11:30 AM C4.05**

**Doping Dependence of Resonant Spin Excitations in BaFe<sub>2</sub>(As<sub>1-x</sub>Px)<sub>2</sub>** Raymond Osborn<sup>1</sup>, John-Paul Castellán<sup>2</sup>, Stephan Rosenkranz<sup>1</sup>, Keith Taddei<sup>1</sup>, Jared Allred<sup>1</sup>, Omar Chmaissem<sup>1</sup>, Sevda Avci<sup>3</sup>, Duck-Young Chung<sup>1</sup>, Helmut Claus<sup>1</sup>, Mercouri Kanatzidis<sup>4,1</sup>, Douglas Abernathy<sup>5</sup> and Matthew Stone<sup>5</sup>; <sup>1</sup>Argonne National Laboratory, Argonne, Illinois; <sup>2</sup>Karlsruhe Institute of Technology, Karlsruhe, Germany; <sup>3</sup>Afyon Kocatepe University, Afyonkarahisar, Turkey; <sup>4</sup>Northwestern University, Evanston, Illinois; <sup>5</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee.

**11:45 AM C4.06**

**Superconductivity and Spin Excitations in Ba(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>2</sub>As<sub>2</sub>** Gregory Tucker<sup>1,2</sup>, D. K. Pratt<sup>1,2</sup>, A. Thaler<sup>1,2</sup>, N. Ni<sup>1,2</sup>, K. Marty<sup>3</sup>, A. D. Christianson<sup>3</sup>, M. D. Lumsden<sup>3</sup>, B. C. Sales<sup>4</sup>, A. S. Sefat<sup>4</sup>, S. L. Bud'ko<sup>1,2</sup>, P. C. Canfield<sup>1,2</sup>, A. I. Goldman<sup>1,2</sup> and R. J. McQueeney<sup>1,2</sup>; <sup>1</sup>Division of Materials Science and Engineering, Ames Laboratory, Ames, Iowa; <sup>2</sup>Department of Physics & Astronomy, Iowa State University, Ames, Iowa; <sup>3</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

**12:00 PM C4.07**

**Magnetic Behavior of the Sawtooth Fe Chains in Rb<sub>2</sub>Fe<sub>2</sub>O(AsO<sub>4</sub>)<sub>2</sub>** Ovidiu Garlea, Quantum Condensed Matter Division, ORNL, Oak Ridge, Tennessee.

SESSION C5: Exotic Phase Transitions in Complex Materials II  
Session Chair: Despina Louca  
Tuesday Afternoon, June 3, 2014  
Summit I

**1:45 PM \*C5.01**

**Collective Magnetic Excitations in Materials with Strong Spin-Orbit Coupling** Young-June Kim<sup>1</sup>, Kemp Plumb<sup>1</sup>, James P. Clancy<sup>1</sup>, A. I. Kolesnikov<sup>2</sup>, B. C. Joon<sup>3</sup>, Tac W. Noh<sup>3</sup>, Ashley Cook<sup>1</sup> and Arun Paramakanti<sup>1</sup>; <sup>1</sup>Physics, University of Toronto, Toronto,

Ontario, Canada; <sup>2</sup>Oak Ridge National Lab, Oak Ridge, Tennessee; <sup>3</sup>Seoul National University, Seoul, Korea, Republic of.

**2:15 PM C5.02**

**Full Magnetic Dispersion Relation in the Frustrated Quasi-1D Ferromagnet Ca<sub>2</sub>Y<sub>2</sub>Cu<sub>5</sub>O<sub>10</sub>** Masaaki Matsuda<sup>1</sup>, Jie Ma<sup>1</sup>, Vasile O. Garlea<sup>1</sup>, Satoshi Nishimoto<sup>2</sup>, Stefan-Ludwig Drechsler<sup>2</sup>, Roman O. Kuzian<sup>3</sup>, Toshimitsu Ito<sup>4</sup>, Hirotaka Yamaguchi<sup>4</sup> and Kunihiro Oka<sup>4</sup>; <sup>1</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Institute for Theoretical Solid State Physics, IFW Dresden, Dresden, Germany; <sup>3</sup>Institute for Problems of Materials Science, NASU, Kiev, Ukraine; <sup>4</sup>National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan.

**2:30 PM C5.03**

**Low Energy Magnetic Excitations and Their Relation to Superconductivity in Ni- and Cu-Doped Fe(Te,Se)** John A. Schneeloch<sup>1,2</sup>, Zhijun Xu<sup>3</sup>, Jinsheng Wen<sup>4</sup>, Masaaki Matsuda<sup>5</sup>, G. E. Granroth<sup>5,6</sup>, Wei Ku<sup>1</sup>, Weiguo Yin<sup>1</sup>, Robert Birgeneau<sup>3,7,8</sup>, Genda Gu<sup>1</sup>, Igor Zaliznyak<sup>1</sup>, John Tranquada<sup>1</sup> and Guangyong Xu<sup>1</sup>; <sup>1</sup>Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York; <sup>2</sup>Physics and Astronomy Department, Stony Brook University, Stony Brook, New York; <sup>3</sup>Physics Department, University of California, Berkeley, California; <sup>4</sup>Center for Superconducting Physics and Materials, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing, China; <sup>5</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>6</sup>Neutron Data Analysis and Visualization Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>7</sup>Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California; <sup>8</sup>Department of Materials Science and Engineering, University of California, Berkeley, California.

**2:45 PM C5.04**

**Weak Increase in Neel Temperature With Pressure in KCuF<sub>3</sub> and Implications for Orbital Order** Alexander Thaler<sup>1</sup>, Andrew D. Christianson<sup>2</sup>, Shi Yuan<sup>1</sup>, Brian Nguyen<sup>1</sup>, Isaac Brodsky<sup>1</sup>, S. L. Cooper<sup>1</sup>, Stephen E. Nagler<sup>2</sup> and Gregory J. MacDougall<sup>1</sup>; <sup>1</sup>Physics Illinois, University of Illinois, Urbana, Illinois; <sup>2</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

**3:00 PM C5.05**

**Multizone Phonon Refinement: A New Tool for Determination of Phonon Spectra** Dan Parshall<sup>1</sup>, R. Heid<sup>2</sup>, Jennifer L. Niedziela<sup>3</sup>, Th. Wolf<sup>2</sup>, M. B. Stone<sup>3</sup>, D. L. Abernathy<sup>3</sup> and D. Reznik<sup>4</sup>; <sup>1</sup>NIST Center for Neutron Research, Gaithersburg, Maryland; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Karlsruhe Institute for Technology, Karlsruhe, Germany; <sup>4</sup>University of Colorado, Boulder, Boulder, Colorado.

**3:15 PM C5.06**

**Localized Bose-Einstein Condensation in Films of Liquid <sup>4</sup>He in Disorder** Henry Glyde<sup>1</sup>, Jacques Bossy<sup>2</sup> and Helmut Schober<sup>3</sup>; <sup>1</sup>Physics, University of Delaware, Newark, Delaware; <sup>2</sup>Institut Neel, CNRS-UJP, Grenoble, France; <sup>3</sup>Institut Laue-Langevin, Grenoble, France.

SESSION CP3: Poster Session III: Hard Condensed Matter  
Tuesday Afternoon, June 3, 2014  
3:30 PM  
Summit II

**CP3.01**

**Nature of Local Distortions in Newly-Discovered Disordered Superconductor, LaO<sub>1-x</sub>FxBiS<sub>2</sub>** Anushika Athauda<sup>1</sup>, Junjie Yang<sup>1</sup>, Despina Louca<sup>1</sup>, Seunghun Lee<sup>1</sup> and Yoshikazu Mizuguchi<sup>2</sup>; <sup>1</sup>University of Virginia, Charlottesville, Virginia; <sup>2</sup>Tokyo Metropolitan University, Tokyo, Japan.

### CP3.02

**Spin Reorientation in the Multiferroic Hexagonal ErMnO<sub>3</sub>**  
Huibo Cao<sup>1</sup>, Jun Zhao<sup>2</sup>, Jic Ma<sup>1</sup>, Tao Hong<sup>1</sup>, Masaaki Matsuda<sup>1</sup> and Bryan Chakoumakos<sup>1</sup>; <sup>1</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Fudan University, Shanghai, China.

### CP3.03

**Exploring the Hidden Order and Large Moment Antiferromagnetic Phase in URu<sub>2-x</sub>Fe<sub>x</sub>Si<sub>2</sub> by Means of Neutron Scattering** Pinaki Das<sup>1</sup>, R. E. Baumbach<sup>1</sup>, E. D. Bauer<sup>1</sup>, M. Janoschek<sup>1</sup>, K. Huang<sup>2</sup>, N. Kanchanavatee<sup>2</sup>, M. B. Maple<sup>2</sup>, Y. Zhao<sup>3</sup>, J. S. Helton<sup>3</sup> and J. Lynn<sup>3</sup>; <sup>1</sup>MPA-CMMS, Los Alamos National Laboratory, Los Alamos, New Mexico; <sup>2</sup>Physics, University of California, San Diego, San Diego, California; <sup>3</sup>NIST Center for Neutron Research, Gaithersburg, Maryland.

### CP3.04

**Raman Scattering (First- and Higher- Order) and Raman Mapping of 2D van der Waals Solids: Graphene and Beyond** E. Heintzman<sup>1</sup>, J. Jasinski<sup>2</sup> and Sanju Gupta<sup>1</sup>; <sup>1</sup>Physics and Astronomy, Western Kentucky University, Bowling Green, Kentucky; <sup>2</sup>Conn Center for Renewable Energy, University of Louisville, Louisville, Kentucky.

### CP3.05

**The Role of Phase-Specific Deformation Behavior in the Compressive Toughness Enhancement of a NiAl-Cr(Mo) Lamellar Composite** Dunji Yu<sup>1</sup>, Hongbin Bei<sup>2</sup>, Yan Chen<sup>1</sup> and Ke An<sup>1</sup>; <sup>1</sup>Chemical and Engineering Materials Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

### CP3.06

**Neutron Spectroscopic Study of Crystal-Field Excitations of Yb<sub>2</sub>(Ti<sub>2-x</sub>Yb<sub>x</sub>)O<sub>7-x/2</sub>** Dalini D. Maharaj<sup>1</sup>, E. Kermarrec<sup>1</sup>, K. A. Ross<sup>2,3</sup>, G. E. Granroth<sup>4</sup>, H. A. Dabkowska<sup>5</sup> and B. D. Gaulin<sup>1,5</sup>; <sup>1</sup>Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada; <sup>2</sup>Institute for Quantum Matter and Department of Physics and Astronomy, John Hopkins University, Baltimore, Maryland; <sup>3</sup>NIST Centre for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland; <sup>4</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratories, Oak Ridge, Tennessee; <sup>5</sup>Brockhouse Institute for Materials Research, McMaster University, Hamilton, Ontario, Canada.

### CP3.07

**On a Bismuth Manganite Film** Daniel M. Pajcrowski<sup>1</sup>, Lisa A. Krayner<sup>1</sup>, Hyoungjeen Jeon<sup>2,3</sup> and Amlan Biswas<sup>3</sup>; <sup>1</sup>NIST, Gaithersburg, Maryland; <sup>2</sup>Physics, Pusan National University, Busan, Korea, Republic of; <sup>3</sup>Physics, University of Florida, Gainesville, Florida.

### CP3.08

**Quasi-Elastic Neutron Scattering Reveals Fast Proton Diffusion in Ca-Doped LaPO<sub>4</sub>** Amal B. Al-Wahish<sup>1</sup>, N. Jalarvo<sup>2</sup>, Z. Bi<sup>3</sup>, C. Bridges<sup>3</sup>, M. P. Paranthaman<sup>3</sup>, A. Huq<sup>2</sup>, K. Herwig<sup>2</sup> and D. Mandrus<sup>1,4,5</sup>; <sup>1</sup>Department of Physics and Astronomy, UTK, Knoxville, Tennessee; <sup>2</sup>Neutron Scattering Sciences Division, ORNL, Oak Ridge, Tennessee; <sup>3</sup>Chemical Sciences Division, ORNL, Oak Ridge, Tennessee; <sup>4</sup>Materials Science and Engineering, UTK, Knoxville, Tennessee; <sup>5</sup>Materials Science and Technology Division, ORNL, Oak Ridge, Tennessee.

### CP3.09

**Doping Influence on the Spin Dynamics and Magnetoelectric Effect in Hexagonal Y<sub>0.7</sub>Lu<sub>0.3</sub>MnO<sub>3</sub>** Wei Tian<sup>1</sup>, Guotai Tan<sup>3,2</sup>, Liu Liu<sup>3</sup>, Jinxing Zhang<sup>3</sup>, Barry Winn<sup>1</sup>, Tao Hong<sup>1</sup>, Fernandez-Baca A. Jaime<sup>1</sup>, Chenglin Zhang<sup>2,4</sup> and Pengcheng Dai<sup>3,4</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>The University of Tennessee, Knoxville, Tennessee; <sup>3</sup>Beijing Normal University, Beijing, China; <sup>4</sup>Rice University, Houston, Texas.

### CP3.10

**Effect of Iron Doping on the Magnetic Structure of U(Ru<sub>1-x</sub>Fe<sub>x</sub>)<sub>2</sub>As<sub>2</sub>** Travis Williams<sup>1</sup>, Adam Aczel<sup>1</sup>, Mark Lumsden<sup>1</sup>, Steve Nagler<sup>1</sup>, Murray Wilson<sup>2</sup> and Graeme Luke<sup>2</sup>; <sup>1</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>McMaster University, Hamilton, Ontario, Canada.

### SESSION C6: Exotic Electronic States

Session Chair: Bruce Gaulin

Wednesday Morning, June 4, 2014

Summit I

### 10:15 AM \*C6.01

#### Frustrated Magnetism with Magnetic Molecules

Martin Mourigal, Johns Hopkins University, Baltimore, Maryland.

### 10:45 AM \*C6.02

**Doping Dependence of the Structural and Magnetic Properties of CeCu<sub>6-x</sub>T<sub>x</sub> (T = Ag, Pd)** Lekhanath Poudel<sup>1,2</sup>, M. McGuire<sup>2</sup>, M. Kochler<sup>1</sup>, C. de la Cruz<sup>2</sup>, S. Calder<sup>2</sup>, W. Tian<sup>2</sup>, M. Matsuda<sup>2</sup>, H. B. Cao<sup>2</sup>, A. Payzant<sup>2</sup>, V. Keppens<sup>1</sup>, D. Mandrus<sup>1,2</sup> and A. D. Christianson<sup>2</sup>; <sup>1</sup>University of Tennessee, Knoxville, Tennessee; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee.

### 11:00 AM C6.03

#### Frangible Antiferromagnetism in the Heavy-Fermion Compound YbBiPt

Benjamin Ueland<sup>1,2</sup>, A. Kreyssig<sup>1,2</sup>, K. Prokes<sup>3</sup>, J. W. Lynn<sup>4</sup>, L. W. Harriger<sup>4</sup>, D. K. Pratt<sup>4</sup>, D. K. Singh<sup>4,5</sup>, T. W. Heitmann<sup>6</sup>, S. Sauerbrei<sup>1,2</sup>, S. M. Saunders<sup>1,2</sup>, E. D. Mun<sup>1,2</sup>, S. L. Bud'ko<sup>1,2</sup>, R. J. McQueeney<sup>1,2</sup>, P. C. Canfield<sup>1,2</sup> and A. I. Goldman<sup>1,2</sup>; <sup>1</sup>Ames Laboratory, Ames, Iowa; <sup>2</sup>Department of Physics and Astronomy, Iowa State University, Ames, Iowa; <sup>3</sup>Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany; <sup>4</sup>NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland; <sup>5</sup>Department of Materials Science and Engineering, University of Maryland, College Park, Maryland; <sup>6</sup>The Missouri Research Reactor, University of Missouri, Columbia, Missouri.

### 11:15 AM C6.04

#### Magnetic Ordering Induced by Interladder Coupling in a Spin-1/2 Heisenberg Two-Leg Ladder Antiferromagnet C<sub>9</sub>H<sub>18</sub>N<sub>2</sub>CuBr<sub>4</sub>

Tao Hong<sup>1</sup>, K. Schmidt<sup>2</sup>, K. Coester<sup>2</sup>, F. Awwadi<sup>3</sup>, M. Turnbull<sup>4</sup>, Y. Qiu<sup>5</sup>, J. Rodriguez-Rivera<sup>5</sup>, M. Zhu<sup>6</sup>, X. Ke<sup>6</sup>, C. Aoyama<sup>7</sup>, Y. Takano<sup>7</sup>, Huibo Cao<sup>1</sup>, W. Tian<sup>1</sup>, J. Ma<sup>1</sup>, R. Custelcean<sup>8</sup>, H. Zhou<sup>9</sup> and M. Matsuda<sup>1</sup>; <sup>1</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>TU Dortmund, Dortmund, Germany; <sup>3</sup>The University of Jordan, Amman, Jordan; <sup>4</sup>Clark University, Worcester, Massachusetts; <sup>5</sup>National Institute of Standards and Technology, Gaithersburg, Maryland; <sup>6</sup>Michigan State University, East Lansing, Michigan; <sup>7</sup>University of Florida, Gainesville, Florida; <sup>8</sup>Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>9</sup>University of Tennessee, Knoxville, Tennessee.

### 11:30 AM C6.05

**Magnetic Excitation Spectrum of the Topological Kondo Insulator SmB<sub>6</sub>** Jonathan Leiner<sup>1</sup>, Wesley Fuhrman<sup>2</sup>, Garrett Granroth<sup>1</sup>, Matt Stone<sup>1</sup>, Mark Lumsden<sup>1</sup>, Lisa DeBeer-Schmitt<sup>1</sup>, Pavel Alekseev<sup>3</sup>, Jean-Michel Mignot<sup>4</sup>, Seyed Koohpayeh<sup>2</sup>, Patrick Cottingham<sup>5</sup>, William Phelan<sup>5</sup>, Leslie Schoop<sup>6</sup>, Robert Cava<sup>6</sup>, Tyrel McQueen<sup>2,5</sup> and Collin Broholm<sup>2,1</sup>; <sup>1</sup>Quantum Condensed Matter Division, Oak Ridge National Lab, Oak Ridge, Tennessee; <sup>2</sup>Department of Physics, Johns Hopkins University, Baltimore, Maryland; <sup>3</sup>Kurchatov Institute, Moscow, Russian Federation; <sup>4</sup>Laboratoire Leon Brillouin, Saclay, France; <sup>5</sup>Department of Chemistry, Johns Hopkins University, Baltimore, Maryland; <sup>6</sup>Department of Chemistry, Princeton University, Princeton, New Jersey.

### 11:45 AM C6.06

**Quantum Oscillations of Light Atoms in UX Salts** Yuen Yiu<sup>1</sup>, Adam Aczel<sup>2</sup>, Jiao Lin<sup>3</sup>, Garrett Granroth<sup>4</sup>, William Buyers<sup>5</sup> and Stephen Nagler<sup>2,6</sup>; <sup>1</sup>Physics and Astronomy, University of Tennessee, Knoxville, Tennessee; <sup>2</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Caltech Center for Advanced Computing Research, California Institute of Technology, Pasadena, California; <sup>4</sup>Neutron Data Analysis and Visualization Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>5</sup>Chalk River Laboratories, Deep River, Ontario, Canada; <sup>6</sup>CIRE, University of Tennessee, Knoxville, Tennessee.

### 12:00 PM C6.07

#### Magnetic Structure and Excitations in Modified Pyrochlore Fluorides ACr<sub>2</sub>F<sub>6</sub> (A=Cs,Rb)

Sachith E. Dissanayake<sup>1</sup>, Seunghun Lee<sup>1</sup>, Yiming Qui<sup>2</sup>, Masaaki Matsuda<sup>3</sup>, Hiroaki Ueda<sup>4</sup> and Andreas Hoser<sup>5</sup>; <sup>1</sup>Department of Physics, University of Virginia, Charlottesville, Virginia; <sup>2</sup>NIST Center for Neutron Research, Gaithersburg, Maryland; <sup>3</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Department of Chemistry, Kyoto University, Kyoto, Japan; <sup>5</sup>Helmholtz Zentrum Berlin, Berlin, Germany.

SESSION C7: Manganites, Cobaltates and Related  
Materials

Session Chair: Chris Leighton  
Wednesday Afternoon, June 4, 2014  
Summit I

1:45 PM **\*C7.01**

**Crossover from Polaronic to Magnetically Phase-Separated Behavior in  $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$**  Daniel Phelan<sup>1</sup>, Sami El-Khatib<sup>2</sup>, Shun Wang<sup>1</sup>, John Barker<sup>3</sup>, Junjing Zhao<sup>4</sup>, Hong Zheng<sup>1</sup>, John Mitchell<sup>4</sup> and Chris Leighton<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, Minnesota; <sup>2</sup>American University of Sharjah, Sharjah, United Arab Emirates; <sup>3</sup>NIST Center for Neutron Research, Gaithersburg, Maryland; <sup>4</sup>Argonne National Laboratory, Lemont, Illinois.

2:15 PM **C7.02**

**Neutron Diffraction Study of the Polarization Reversal in Multiferroic  $\text{Mn}_{0.85}\text{Co}_{0.15}\text{WO}_4$  Induced by An External Magnetic Field** Feng Ye<sup>1</sup>, Songxue Chi<sup>1</sup>, Masaaki Matsuda<sup>1</sup>, Jaime A. Fernandez-Baca<sup>1</sup>, N. Poudel<sup>2</sup>, Bernd Lorenz<sup>2</sup>, K. C. Liang<sup>2</sup>, Y. Q. Wang<sup>2</sup>, Y. Y. Sun<sup>2</sup> and C. W. Chu<sup>2</sup>; <sup>1</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Knoxville, Tennessee; <sup>2</sup>Department of Physics, University of Houston, Houston, Texas.

2:30 PM **C7.03**

**Magnetic Structure of Bulk Hexagonal  $\text{LuFe}(1-x)\text{Mn}(x)\text{O}_3$**  Steven M. Disseler<sup>1</sup>, William Ratcliff<sup>1</sup>, Yoon Seok Oh<sup>2</sup>, Jeffrey Lynn<sup>1</sup> and Sang W. Cheong<sup>2</sup>; <sup>1</sup>NIST Center for Neutron Research, Gaithersburg, Maryland; <sup>2</sup>Physics, Rutgers University, Piscataway, New Jersey.

2:45 PM **C7.04**

**Exotic Magnetism on the Quasi-Fcc Lattices of the D3 Double Perovskites  $\text{La}_2\text{NaB}'\text{O}_6$  ( $\text{B}' = \text{Ru, Os}$ )** Adam Aczel<sup>1</sup>, Peter Baker<sup>2</sup>, Daniel Bugaris<sup>3</sup>, Jeongho Yeon<sup>3</sup>, Hanno zur Loye<sup>3</sup>, Tatiana Guidi<sup>2</sup> and D. T. Adroja<sup>2</sup>; <sup>1</sup>Quantum Condensed Matter, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>ISIS Facility, Rutherford Appleton Laboratory, Harwell Oxford, United Kingdom; <sup>3</sup>Chemistry and Biochemistry, University of South Carolina, Columbia, South Carolina.

3:00 PM **C7.05**

**Discovery of New Magnetic Excitations in Nickel Metal** Herb Mook<sup>1</sup>, Toby Perring<sup>3</sup> and Stephen Hayden<sup>2</sup>; <sup>1</sup>Neutron Sciences Directorate, ORNL, Oak Ridge, Tennessee; <sup>2</sup>H.H. Wills Physics Laboratory, University of Bristol Laboratory, Bristol BSB TTL, United Kingdom; <sup>3</sup>ISIS Facility, Rutherford Appleton, Chilton, United Kingdom.

3:15 PM **C7.06**

**Anisotropic Phonon Dynamics and Thermal Transport in Thermoelectric  $\text{CrSb}_2$**  Chen Li<sup>1</sup>, Olivier Delaire<sup>1</sup>, Matt Stone<sup>2</sup>, Andrew May<sup>1</sup> and Brian Sales<sup>1</sup>; <sup>1</sup>Material Science and Technology Division, Oak Ridge National Laboratory, Knoxville, Tennessee; <sup>2</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

3:30 PM **BREAK**

SESSION C8: Superconductivity and Related Materials  
Session Chair: Raymond Osborn  
Wednesday Afternoon, June 4, 2014  
Summit I

4:00 PM **C8.01**

**Temperature and Doping Evolution of Magnetic Scattering in Non-Superconducting  $\text{Fe}_{1+y}\text{Te}$  and Superconducting  $\text{FeTe}_{1-x}(\text{S,Se})_x$**  Igor Zaliznyak<sup>1</sup>, Zhijun Xu<sup>1</sup>, Genda Gu<sup>1</sup>, John Tranquada<sup>1</sup>, Cedomir Petrovic<sup>1</sup>, Rongwei Hu<sup>1</sup>, Andrei Savici<sup>2</sup>, Mark Lumsden<sup>2</sup> and Matthew Stone<sup>2</sup>; <sup>1</sup>CMPMSD, Brookhaven National Laboratory, Upton, New York; <sup>2</sup>NSSD, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

4:15 PM **C8.02**

**Observation of An Acoustic Mode Potentially Driven by An Imbalance Between the Magnetic Moments of Neighboring Fe Atoms in  $\text{Fe}_{1+y}\text{Te}$  ( $y < 0.12$ )** David Fobes<sup>1</sup>, Igor Zaliznyak<sup>1</sup>, Zhijun Xu<sup>1,2</sup>, Genda Gu<sup>1</sup>, John M. Tranquada<sup>1</sup>, Xu-Gang He<sup>1</sup>, Wei Ku<sup>1</sup> and Ovidiu Garlea<sup>3</sup>; <sup>1</sup>CMPMSD, Brookhaven National Laboratory, Upton, New York; <sup>2</sup>Department of Physics, University of California, Berkeley, California; <sup>3</sup>QCMD, Oak Ridge National Lab, Oak Ridge, Tennessee.

4:30 PM **C8.03**

**The Structural and Magnetic Properties of  $\text{CsxFe}_{2-y}\text{Se}_2$  as Determined by X-Ray and Neutron Scattering of Powder and Single Crystal Samples** Keith M. Taddei<sup>1</sup>, Mihai Sturza<sup>3</sup>, Sevda Avci<sup>4</sup>, Omar Chmaissem<sup>1</sup>, Stephan Rosenkranz<sup>3</sup>, Ray Osborn<sup>3</sup>, Mercouri Kanatzidis<sup>2,3</sup> and Duck Chung<sup>1</sup>; <sup>1</sup>Physics, Northern Illinois University, DeKalb, Illinois; <sup>2</sup>Northwestern University, Evanston, Illinois; <sup>3</sup>Argonne National Laboratory, Lemont, Illinois; <sup>4</sup>Afyon Kocatepe University, Afyon, Turkey.

4:45 PM **C8.04**

**Spin-Phonon Hybridization in 214 La-Based Superconductors** Jerod Wagman<sup>1</sup>, J. P. Carlo<sup>2</sup>, G. van Gastel<sup>1</sup>, M. B. Stone<sup>3</sup>, J. L. Niedziela<sup>3</sup>, G. E. Granroth<sup>3</sup>, A. I. Kolesnikov<sup>3</sup>, L. DeBeer-Schmitt<sup>3</sup>, A. T. Savici<sup>3</sup>, Z. Yamani<sup>4</sup>, Z. Tun<sup>4</sup>, Yang Zhao<sup>5,6</sup>, A. B. Kallin<sup>7</sup>, E. Mazurek<sup>8</sup>, H. A. Dabkowska<sup>8</sup> and B. D. Gaulin<sup>1,8,9</sup>; <sup>1</sup>McMaster University, Hamilton, Ontario, Canada; <sup>2</sup>Villanova University, Villanova, Pennsylvania; <sup>3</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Chalk River Laboratories, Chalk River, Ontario, Canada; <sup>5</sup>University of Maryland, College Park, Maryland; <sup>6</sup>National Institute of Standards and Technology, Gaithersburg, Maryland; <sup>7</sup>University of Waterloo, Waterloo, Ontario, Canada; <sup>8</sup>Brockhouse Institute of Materials Research, Hamilton, Ontario, Canada; <sup>9</sup>Canadian Institute for Advanced Research, Toronto, Ontario, Canada.

5:00 PM **C8.05**

**Exotic Magnetism on the FCC Lattice of 5d Double Perovskites** Edwin Kermarrec<sup>1</sup>, Dalini Maharaj<sup>1</sup>, Casey Marjerrison<sup>2</sup>, Corey Thompson<sup>2</sup>, Jeremy Carlo<sup>3</sup>, Patrick Clancy<sup>4</sup>, Garrett Granroth<sup>5</sup>, John Greedan<sup>2</sup>, Hanna Dabkowska<sup>8</sup> and Bruce Gaulin<sup>1,6,7</sup>; <sup>1</sup>Physics & Astronomy, McMaster University, Hamilton, Ontario, Canada; <sup>2</sup>Chemistry, McMaster University, Hamilton, Ontario, Canada; <sup>3</sup>Physics, Villanova University, Villanova, Pennsylvania; <sup>4</sup>Physics, University of Toronto, Toronto, Ontario, Canada; <sup>5</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>6</sup>Brockhouse Institute for Materials Research, Hamilton, Ontario, Canada; <sup>7</sup>Canadian Institute for Advanced Research, Toronto, Ontario, Canada.

5:15 PM **C8.06**

**Atomic Distributions in Multi-Principal Element Alloys** Louis J. Santodonato<sup>1,2</sup>, Mikhail Feygenson<sup>3</sup>, Joerg C. Neuefeind<sup>3</sup>, Yang Zhang<sup>4</sup> and Peter K. Liaw<sup>2</sup>; <sup>1</sup>Instrument and Source Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Materials Science and Engineering, The University of Tennessee, Knoxville, Tennessee; <sup>3</sup>Chemical and Engineering Materials Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Department of Nuclear, Plasma, and Radiological Engineering, The University of Illinois at Urbana-Champaign, Urbana, Illinois.

SESSION CP4: Poster Session IV: Hard Condensed  
Matter  
Wednesday Evening, June 4, 2014  
5:30 PM  
Summit II

**CP4.01**

**Structure and Dynamics of the Proton Conductor, Ca/Sr-doped  $\text{LaPO}_4$**  Amal B. Al-Wahish<sup>1</sup>, C. Bridges<sup>2</sup>, U. al-Binni<sup>3</sup>, Z. Bi<sup>2</sup>, A. Huq<sup>4</sup>, S. Tang<sup>5</sup>, L. Tetard<sup>6</sup>, M. P. Paranthaman<sup>2</sup>, D. Mandrus<sup>1,5,7</sup>; <sup>1</sup>Department of Physics and Astronomy, UTK, Knoxville, Tennessee; <sup>2</sup>Chemical Sciences Division, ORNL, Knoxville, Tennessee; <sup>3</sup>Department of Physics, Astronomy and Geology, Berry College, Mt. Berry, Georgia; <sup>4</sup>Spallation Neutron Source (SNS), ORNL, Knoxville, Tennessee; <sup>5</sup>Materials Science and Engineering, UTK, Knoxville, Tennessee; <sup>6</sup>NanoScience Technology Center-University of Central Florida, Orlando, Florida; <sup>7</sup>Materials Science and Technology Division, ORNL, Knoxville, Tennessee.

**CP4.02**

**Neutron and X-Ray Scattering Studies of Anharmonic Phonons in  $\text{VO}_2$**  John D. Budai<sup>1</sup>, Jiawang Hong<sup>1</sup>, Olivier Delaire<sup>1</sup>, Michael Manley<sup>1</sup>, Eliot Specht<sup>1</sup>, Chen Li<sup>1</sup>, Douglas Abernathy<sup>2</sup>, Jon Tischler<sup>3</sup>, Ayman Said<sup>3</sup>, Robert McQueeney<sup>2</sup> and Lynn Boatner<sup>1</sup>; <sup>1</sup>Materials Science & Technology, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Neutron Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois.

**CP4.03**

**Incommensurate Magnetic Ordering in  $\text{HgCr}_2\text{S}_4$**  Naveen K. Chogondahalli Muniraju<sup>1</sup>, Michael Ohl<sup>1</sup>, Vladimir Tsurkan<sup>2</sup> and Peter Lunkenheimer<sup>2</sup>; <sup>1</sup>Juelich Center for Neutron Science (JCNS), Forschungszentrum Juelich, Oak Ridge, Tennessee; <sup>2</sup>Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany.

#### **CP4.04**

**Low-Temperature Thermometry Calibration Station at the SNS** Todd E. Sherline, Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### **CP4.05**

**Large Anharmonicity in Complex Oxides from *Ab Initio* Molecular Dynamics Simulations** Jiawang Hong, Olivier Delaire, John Budai, Michael Manley, Chen Li and Eliot Specht; Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### **CP4.06**

**Phonon Anharmonicity in Silicon** Dennis S. Kim<sup>1</sup>, Hillary L. Smith<sup>1</sup>, Jennifer L. Niedziela<sup>2</sup>, Doug L. Abernathy<sup>3</sup> and Brent T. Fultz<sup>4</sup>; <sup>1</sup>Applied Physics and Materials Science, California Institute of Technology, Pasadena, California; <sup>2</sup>Instrument and Source Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### **CP4.07**

**Layer-Resolved Magnetization Depth Profile of Annealed CoFeB/MgO Multilayer** Ki-Yeon Kim<sup>1,3</sup>, Byoung-Chul Min<sup>2</sup>, Jong Kahk Keum<sup>3</sup>, Sin-Yong Jo<sup>4</sup>, Chun-Yeol You<sup>4</sup>, S. Park<sup>5</sup>, Haile Ambaye<sup>3</sup> and Valeria Lauter<sup>3</sup>; <sup>1</sup>Korea Atomic Energy Research Institute, Daejeon, Korea, Republic of; <sup>2</sup>Korea Institute of Science and Technology, Seoul, Korea, Republic of; <sup>3</sup>Oak Ridge National Laboratory, Knoxville, Tennessee; <sup>4</sup>Inha University, Incheon, Korea, Republic of; <sup>5</sup>Pusan National University, Busan, Korea, Republic of.

#### **CP4.08**

**Design of a High Field Pulsed Magnet at SNS** Jooseop Lee, Justin R. Carmichael, Gerald M. Rucker and Garrett E. Granroth; Oak Ridge National Lab, Oak Ridge, Tennessee.

#### **CP4.09**

**Determination of the Magnetic Structure of a New Post-Spinel Compound LaSbCo<sub>2</sub>O<sub>6</sub>** Kuo Li<sup>1,2,3</sup>, Yingxia Wang<sup>2</sup> and Jianhua Lin<sup>2</sup>; <sup>1</sup>Geophysical Lab, Carnegie Institution of Washington, Oak Ridge, Tennessee; <sup>2</sup>Peking University, Beijing, China; <sup>3</sup>Center for High Pressure Science and Technology Advanced Research, Beijing, China.

SESSION C9: Magnetic Nanostructures and Thin Films  
Session Chair: Yaohua Liu  
Thursday Morning, June 5, 2014  
Summit I

#### **9:45 AM \*C9.01**

**Roles of Surfactant Coating and Magnetocrystalline Anisotropy on Magnetic Nanoparticle Response** Kathryn L. Krycka<sup>1</sup>, Yumi Ijiri<sup>2</sup>, Priscyla Andrade<sup>3</sup>, Ryan Booth<sup>4</sup>, Julie A. Borchers<sup>1</sup>, Kathryn Hasz<sup>2</sup>, James J. Rhyne<sup>5</sup>, Samuel Oberdick<sup>4</sup>, Jucelino Leao<sup>1</sup>, J. A. Aguiar<sup>3</sup> and Sara A. Majetich<sup>4</sup>; <sup>1</sup>NIST Center for Neutron Research, Gaithersburg, Maryland; <sup>2</sup>Physics, Oberlin College, Oberlin, Ohio; <sup>3</sup>Universidade Federal de Pernambuco, Recife, Brazil; <sup>4</sup>Physics, Carnegie Mellon University, Pittsburgh, Pennsylvania; <sup>5</sup>U.S. Department of Energy, Washington, D.C., District of Columbia.

#### **10:15 AM C9.02**

**Investigation of An Intrinsic Room Temperature Ferromagnetism Through Spectroscopic Studies on Co Doped ZnO Nano Particles** Srinatha Narayanaswamy<sup>1</sup>, Basavaraj Angadi Angadi<sup>1</sup>, K. G. Nair<sup>2</sup>, Y. C. Shao<sup>3</sup>, Nishad G. Deshpande<sup>3</sup> and Way F. Pong<sup>3</sup>; <sup>1</sup>Department of Physics, Bangalore University, Bangalore, Karnataka, India; <sup>2</sup>UGC-DAE CSR, Kalpakkam Node, Kalpakkam, Tamil Nadu, India; <sup>3</sup>Department of Physics, Tamkang University, Tamsui, Taipei, Taiwan.

#### **10:30 AM C9.03**

**Probing Domain Structure in High-Density Segmented Nanowire Arrays Through Polarization Analyzed SANS** Alexander Grutter<sup>1</sup>, Kathryn Krycka<sup>1</sup>, Julie Borchers<sup>1</sup>, Jung Jin Park<sup>2</sup>, Olena Tartakivska<sup>3</sup>, Madhukar Reddy<sup>4</sup>, Brian Kirby<sup>1</sup>, Eliot Estrine<sup>4</sup>, Alison Flatau<sup>2</sup> and Bethanie Stadler<sup>2</sup>; <sup>1</sup>NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland; <sup>2</sup>Department of Aerospace Engineering, University of Maryland, College Park, Maryland; <sup>3</sup>Institute of Magnetism, National Academy of Sciences of Ukraine, Kiev, Ukraine; <sup>4</sup>Electrical and Computer Engineering, University of Minnesota, Minneapolis, Minnesota.

#### **10:45 AM C9.04**

**Ordering of Magnetic Nanoparticles in a Ferrofluid in Contact to a Solid Surface** Katharina Theis-Brochl<sup>1</sup>, Philipp Gutfreund<sup>2</sup>, Max Wolff<sup>3</sup>, Alexei Vorobiev<sup>3</sup> and Boris Toperverg<sup>4</sup>; <sup>1</sup>University of Applied Sciences Bremerhaven, Bremerhaven, Germany; <sup>2</sup>Institut Laue-Langevin, Grenoble, France; <sup>3</sup>Department of Physics and Astronomy, Materials Physics, Uppsala, Sweden; <sup>4</sup>Department of Physics and Astronomy, Ruhr-University Bochum, Bochum, Germany.

#### **11:00 AM C9.05**

**Heterostructure of a Topological Insulator and a Ferromagnetic Insulator Bi-Layer: Spatial Characterization with Polarized Neutron Scattering** Valeria Lauter<sup>1</sup>, Ferhat Katmis<sup>2</sup>, Pablo Jarillo-Herrero<sup>2</sup>, Jagadeesh S. Moodera<sup>2</sup>, Badih Assaf<sup>3</sup> and Don Heiman<sup>3</sup>; <sup>1</sup>NSSD, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Francis Bitter Magnet Lab, MIT, Cambridge, Massachusetts; <sup>3</sup>Department of Physics, Northeastern University, Boston, Massachusetts.

#### **11:15 AM C9.06**

**Emergent Spin-Filter at the Interface Between Ferromagnetic and Insulating Layered Oxides** Yaohua Liu<sup>1</sup>, F. A. Cuellar<sup>2</sup>, Z. Sefrioui<sup>2</sup>, J. W. Freeland<sup>3</sup>, M. R. Fitzsimmons<sup>4</sup>, C. Leon<sup>2</sup>, J. Santamaria<sup>2</sup> and S. G. te Velthuis<sup>1</sup>; <sup>1</sup>Materials Science Division, Argonne National Laboratory, Lemont, Illinois; <sup>2</sup>GFMC, Departamento de Fisica Aplicada III, Universidad Complutense de Madrid, Campus Moncloa, Madrid, Madrid, Spain; <sup>3</sup>Advanced Photon Source, Argonne National Laboratory, Lemont, Illinois; <sup>4</sup>Los Alamos National Laboratory, Los Alamos, New Mexico.

#### **11:30 AM C9.07**

**Discrete Helicoidal States in Thin MnSi Films** Helmut Fritzsche<sup>1</sup>, Murray N. Wilson<sup>2</sup>, Eric A. Karhu<sup>2</sup>, David P. Lake<sup>2</sup>, Andrew S. Quigley<sup>2</sup>, Simon Meynell<sup>2</sup>, Alex N. Bogdanov<sup>3</sup>, Ulrich Roessler<sup>3</sup> and Theodore L. Monchesky<sup>2</sup>; <sup>1</sup>Canadian Neutron Beam Centre, Atomic Energy of Canada Limited, Chalk River, Ontario, Canada; <sup>2</sup>Department of Physics and Atmospheric Science, Dalhousie University, Halifax, Nova Scotia, Canada; <sup>3</sup>Leibniz Institute for Solid State and Materials Research, Dresden, Saxony, Germany.



# D: Soft Matter

SESSION D1: Soft Matter under Flow  
Session Chair: Matthew Helgeson  
Monday Morning, June 2, 2014  
Tennessee Ballroom A

\* Invited paper

SESSION DP1: Poster Session I: Soft Matter  
Sunday Evening, June 1, 2014  
5:00 PM  
Summit II

## DP1.01

**Structural Evolution of Polylactide Molecular Brushes: Kinetics Study by Size Exclusion Chromatography, Neutron Scattering and Simulations** Suk-kyun Ahn<sup>1</sup>, Jan-Michael Carrillo<sup>2</sup>, Youngkyu Han<sup>3</sup>, Taehwan Kim<sup>4</sup>, Kunlun Hong<sup>1</sup> and Changwoo Do<sup>3</sup>; <sup>1</sup>Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Biology and Soft Matter Division, Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Neutron Science Division, Research Reactor Utilization Department, Korea Atomic Energy Research Institute, Daejeon, Korea, Republic of.

## DP1.02

**Molecular Dynamics Simulations and Neutron Scattering Studies for Bottlebrush Polymers** Zhe Zhang<sup>1</sup>, Suk-kyun Ahn<sup>2</sup>, Jan-Michael Carrillo<sup>3</sup>, Bin Wu<sup>4</sup>, Kunlun Hong<sup>2</sup>, Gregory Smith<sup>1</sup> and Changwoo Do<sup>1</sup>; <sup>1</sup>Biology and Soft Matter Division, Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Department of Physics and Astronomy, Joint Institute for Neutron Science, University of Tennessee, Knoxville, Tennessee.

## DP1.03

**Effects of Composition and Temperature on Side-Chain Dynamics of P3HT:PCBM Blends: A Quasi Elastic Neutron Scattering Study** Thusitha N. Etampawala<sup>1</sup>, Dilru R. Ratnaweera<sup>1</sup>, Brian Morgan<sup>1</sup>, Souleymane O. Diallo<sup>2</sup>, Eugene Mamontov<sup>2</sup> and Mark Daddmun<sup>1,2</sup>; <sup>1</sup>Chemistry, University of Tennessee, Knoxville, Tennessee; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## DP1.04

**The Nanoscale Morphology of p-DTS(FBTTh2)2: PC70BM Photovoltaic Films** Nuradhika Herath<sup>1</sup>, Valeria Lauter<sup>1</sup>, Jim Browning<sup>2</sup>, Jong K. Keum<sup>3</sup>, Iliia N. Ivanov<sup>3</sup>, Jiahua Zhu<sup>3</sup> and Kai Xiao<sup>3</sup>; <sup>1</sup>Quantum Condensed Matter Division, Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Chemical and Engineering Material Division, Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## DP1.05

**Orientation Order in Dense Highly Charged Polyelectrolyte Solutions** Philippe Lorchat<sup>1</sup>, Jérôme Combet<sup>2</sup>, Andre Laschewsky<sup>3</sup>, Albert Johner<sup>2</sup>, Sergei Obukhov<sup>4</sup> and Michel Rawiso<sup>2</sup>; <sup>1</sup>Chemistry Department, University of North Carolina, Chapel Hill, North Carolina; <sup>2</sup>Institut Charles Sadron CNRS- Université de Strasbourg, Strasbourg, Alsace, France; <sup>3</sup>Fraunhofer Institut fuer Angewandte Polymerforschung, Postdam, Germany; <sup>4</sup>Physics Department, University of Florida, Gainesville, Florida.

## DP1.06

**Structure of Micellar Water Solutions of Nonionic Gemini Surfactant Study by Small Angle Neutron Scattering Method** Aldona Rajewska<sup>1</sup> and Kazimiera A. Wilk<sup>2</sup>; <sup>1</sup>National Center for Nuclear Research, Swierk-Otwock, Poland; <sup>2</sup>Department of Chemistry, Wroclaw University of Technology, Wroclaw, Poland.

## DP1.07

**Structure and Conformation of Conjugated Ionic Polymers** Sidath Wijesinghe<sup>1</sup>, Naresh C. Osti<sup>1</sup>, Thusitha Etampawala<sup>1</sup>, Dvora Perahia<sup>1</sup> and Gary S. Grest<sup>2</sup>; <sup>1</sup>Chemistry, Clemson University, Clemson, South Carolina; <sup>2</sup>Sandia National Laboratories, Albuquerque, New Mexico.

## 10:15 AM \*D1.01

**Spatiotemporal SANS Measurements of Microstructure Evolution in Dynamically Sheared Polymer-Like Micellar Solutions** A. Kate Gurnon<sup>1</sup>, Carlos Lopez-Barron<sup>1</sup>, Aaron P. Eberle<sup>2</sup>, Lionel Porcar<sup>3</sup> and Norman J. Wagner<sup>1</sup>; <sup>1</sup>Center for Neutron Science, Dept. of Chemical & Biomolecular Engineering, University of Delaware, Newark, Delaware; <sup>2</sup>NCNR NIST, Gaithersburg, Maryland; <sup>3</sup>Institut Laue-Langevin, Grenoble, France.

## 10:45 AM D1.02

**Molecular Behavior of Entangled Polymers in a Non-Linear Rheological Domain** Eric J. Yearley<sup>1</sup>, Leslie A. Sasa<sup>2,1</sup> and Rex P. Hjelm<sup>1</sup>; <sup>1</sup>Los Alamos Neutron Science Center, Los Alamos National Laboratory, Los Alamos, New Mexico; <sup>2</sup>Department of Mechanical Engineering, University of California, Los Angeles, California.

## 11:00 AM D1.03

**The Effect of Shear Flow and Magnetic Field on the Anisotropy and the Size of  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> Nanoparticle Clusters in Magnetic Inks** Jessica Hong and Krishnamurthy Vemuru; School of Physics, Astronomy, Computational Sciences, George Mason University, Fairfax, Virginia.

## 11:15 AM D1.04

**Shear-Induced Microstructure and Rheology of Linear and Branched Wormlike Micelles** Jason P. Rich<sup>1</sup>, Michael R. Weaver<sup>2</sup>, Katie M. Weigandt<sup>3</sup> and Gregory S. Smith<sup>1</sup>; <sup>1</sup>Neutron Sciences Directorate, Soft Matter and Biology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Corporate Research and Development, Analytical Sciences, Procter and Gamble, Mason, Ohio; <sup>3</sup>NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland.

## 11:30 AM D1.05

**Developing Spatiotemporally-Resolved Small Angle Neutron Scattering (STR-SANS) Techniques to Characterize Branching in Wormlike Micellar Solutions Under Nonlinear Shear Flows** Michelle Calabrese, Simon Rogers and Norman J. Wagner; Chemical and Biomolecular Engineering, University of Delaware, Newark, Delaware.

## 11:45 AM D1.06

**Removing Defects in Poly(3-hexylthiophene) Fibrils by Flow** Ngoc A. Nguyen<sup>1</sup>, Hao Shen<sup>2</sup>, Roddel Remy<sup>1</sup>, Yun Liu<sup>2,3</sup> and Michael E. Mackay<sup>1,2</sup>; <sup>1</sup>Materials Science and Engineering, University of Delaware, Newark, Delaware; <sup>2</sup>Chemical and Biomolecular Engineering, University of Delaware, Newark, Delaware; <sup>3</sup>Center for Neutron Scattering, The National Institute of Standards and Technology, Gaithersburg, Maryland.

SESSION D2: Polymer Systems  
Session Chair: Alan Nakatani  
Monday Afternoon, June 2, 2014  
Tennessee Ballroom A

## 1:45 PM \*D2.01

**Neutron Scattering Measurements of Polymer Radius of Gyration in Polymer Nanocomposites** Michael K. Crawford<sup>1</sup>, Robert J. Smalley<sup>1</sup>, Gordon M. Cohen<sup>1</sup>, Barbara L. Hogan<sup>1</sup>, Barbara A. Wood<sup>1</sup>, Sanat K. Kumar<sup>2</sup>, Yuri B. Melnichenko<sup>3</sup>, William E. Guise<sup>1,4</sup> and Boualem Hammouda<sup>5</sup>; <sup>1</sup>Central Research & Development, DuPont Company, Wilmington, Delaware; <sup>2</sup>Chemical Engineering, Columbia University, New York, New York; <sup>3</sup>Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Advanced Photon Source, Argonne National Laboratory, Lemont, Illinois; <sup>5</sup>NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland.

## 2:15 PM D2.02

**Dynamic Caging of Ppolymer Chains in PMMA/SWNT Composites** Rana Ashkar<sup>1,2</sup>, Mansour Abdulbaki<sup>3</sup>, Madhusudan Tyagi<sup>1</sup>, Antonio Faraone<sup>1</sup>, Paul Butler<sup>1</sup> and Ramanan Krishnamoorti<sup>3</sup>; <sup>1</sup>NCNR, NIST, Gaithersburg, Maryland; <sup>2</sup>Materials Science & Engineering Dept., University of Maryland, College Park, Maryland; <sup>3</sup>Dept. of Chemical Engineering, University of Houston, Houston, Texas.

**2:30 PM D2.03**

**Microscopic Dynamics in Nano-Composites of Poly(ethylene oxide) and Poly(methyl methacrylate) Soft Nano-Particles: A Quasi-Elastic Neutron Scattering Study** Debsindhu Bhowmik<sup>1,2</sup>, J. Pomposo<sup>3,4,5</sup>, A. Arbe<sup>3</sup> and J. Colmenero<sup>2,3,4</sup>; <sup>1</sup>Physics, Wayne State University, Detroit, Michigan; <sup>2</sup>Donostia International Physics Center, San Sebastian, Spain; <sup>3</sup>Centro de Fisica de Materiales (CSIC-UPV/EHU) –Materials Physics Center (MPC), San Sebastian, Spain; <sup>4</sup>Departamento de Fisica de Materiales (UPV/EHU), San Sebastian, Spain; <sup>5</sup>IKERBASQUE -Basque Foundation for Science, Bilbao, Spain.

**2:45 PM D2.04**

**Probing the Interlamellar Amorphous Phase in Semicrystalline Polyolefins Using Vapor-Flow Small-Angle Neutron Scattering** Amanda G. McDermott<sup>1</sup>, Chad R. Snyder<sup>1</sup>, Paul J. DesLauriers<sup>2</sup> and Ronald L. Jones<sup>1</sup>; <sup>1</sup>Materials Science and Engineering Division, National Institute of Standards and Technology, Gaithersburg, Maryland; <sup>2</sup>Chevron Phillips Chemical Company LP, Bartlesville, Oklahoma.

**3:00 PM D2.05**

**Polymer Gel Structure in the Collapsed Phase by Molecular Imprinting** Kimani A. Stancil and Charlezetta E. Stokes; Physics and Astronomy, Howard University, Washington, District of Columbia.

**3:15 PM D2.06**

**Polymer Local Dynamics Under Cylindrical Nano-Confinement** Wei-Shao Tung<sup>1</sup>, Nigel Clarke<sup>3</sup>, Karen Winey<sup>1</sup>, Russ Composto<sup>1</sup> and Robert Riggeman<sup>2</sup>; <sup>1</sup>Materials Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania; <sup>2</sup>Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, Pennsylvania; <sup>3</sup>Physics and Astronomy, University of Sheffield, Sheffield, United Kingdom.

**3:30 PM BREAK**

SESSION D3: Membrane and Thin Film Systems  
Session Chair: Michael Mackay  
Monday Afternoon, June 2, 2014  
Tennessee Ballroom A

**4:00 PM \*D3.01**

**Polyelectrolyte Multilayers as a Platform for pH-Responsive Lipid Bilayers** Ann Junghans, Saurabh Singh and Jaroslav Majewski; Lujan Center, LANL, Los Alamos, New Mexico.

**4:30 PM D3.02**

**Thickness Fluctuations Revealed by Neutron Spin Echo** Michihiro Nagao<sup>1,2</sup>, Rana Ashkar<sup>1,3</sup>, Robert Bradbury<sup>1,2</sup>, Andrea Woodka<sup>4</sup> and Paul D. Butler<sup>1,5</sup>; <sup>1</sup>Center for Neutron Research, Natl Inst of Standards & Tech, Gaithersburg, Maryland; <sup>2</sup>Department of Physics, Indiana University, Bloomington, Indiana; <sup>3</sup>University of Maryland, College Park, Maryland; <sup>4</sup>United States Military Academy, West Point, New York; <sup>5</sup>University of Delaware, Newark, Delaware.

**4:45 PM D3.03**

**Using Neutron Reflectivity to Study the Effect of Soft Nanoparticles on the Diffusion of Polystyrene in a Nanocomposite** Adam Imcl<sup>1</sup>, Brad Miller<sup>1</sup>, Wade Holly<sup>2</sup>, Durairaj Baskaran<sup>1</sup> and Mark Dadmun<sup>1,2</sup>; <sup>1</sup>Chemistry, University of Tennessee, Knoxville, Tennessee; <sup>2</sup>Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

**5:00 PM D3.04**

**The Effect of Layering on pH-Triggered Swelling of Nanothin Hydrogels** John F. Ankner<sup>1</sup>, Oleksandra Zavgorodnya<sup>2</sup>, Veronika Kozlovskaya<sup>2</sup> and Eugenia Kharlampieva<sup>2</sup>; <sup>1</sup>Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Dept. of Chemistry, U. of Alabama at Birmingham, Birmingham, Alabama.

**5:15 PM D3.05**

**Estimation of Bilayer Membrane Thicknesses, Fluctuation Amplitudes, and Membrane Wavelength Through Small-Angle Scattering Profiles** Takumi Hara and Victor Lee; Aerospace and Mechanical Engineering, University of Oklahoma, Norman, Oklahoma.

SESSION DP2: Poster Session II: Soft Matter  
Monday Evening, June 2, 2014  
5:30 PM  
Summit II

**DP2.01**

**Thin Films of Lamellar Forming Polydisperse Di-Block Copolymers** John F. Ankner<sup>1</sup>, Rajeev Kumar<sup>2,3</sup>, Bradley S. Lokitz<sup>3</sup>, Bobby G. Sumpter<sup>3</sup>, Scott W. Sides<sup>4</sup> and S. M. Kilbey<sup>5</sup>; <sup>1</sup>Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>National Renewable Energy Laboratory, Golden, Colorado; <sup>5</sup>Dept. of Chemistry, U. of Tennessee, Knoxville, Tennessee.

**DP2.02**

**Morphology Development During Deposition in OPV with Low Band Gap Polymer:Bis-Fullerene Heterojunctions: Effect of a Second Solvent** Huipeng Chen<sup>1</sup>, Yu-Che Hsiao<sup>2</sup>, Jihua Chen<sup>3</sup>, Bin Hu<sup>2</sup> and Mark Dadmun<sup>1,4</sup>; <sup>1</sup>Chemistry, University of Tennessee, Knoxville, Tennessee; <sup>2</sup>Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee; <sup>3</sup>Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

**DP2.03**

**Dynamics of Ion Containing Polymers using Molecular Dynamics Simulation** Monojoy Goswami, Bobby G. Sumpter and Jose M. Borreguero Calvo; Oak Ridge National Laboratory, Oak Ridge, Tennessee.

**DP2.04**

**Elucidating the Impact of Side Chains on the Self-Assembly Behaviors of Poly(3-hexylthiophene) Derivatives by Scattering Techniques** Kunlun Hong<sup>1</sup>, Changwoo Do<sup>2</sup>, Lilin He<sup>2</sup>, Jong Keum<sup>2</sup> and Kunlun Hong<sup>1</sup>; <sup>1</sup>Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

**DP2.05**

**Investigation of Pretreatment-Specific Changes in Biomass Structure** Loukas Petridis<sup>1</sup>, Sai Venkatesh Pingali<sup>1</sup>, Daisuke Sawada<sup>1</sup>, Volker Urban<sup>1</sup>, Hugh M. O'Neill<sup>1</sup>, Garima Bali<sup>2</sup>, Arthur Ragauskas<sup>2</sup>, Barbara Evans<sup>1</sup>, Jeremy Smith<sup>1</sup>, Brian Davison<sup>1</sup> and Paul Langan<sup>1</sup>; <sup>1</sup>ORNL, Oak Ridge, Tennessee; <sup>2</sup>Georgia Institute of Technology, Atlanta, Georgia.

**DP2.06**

**Dynamics of a Liquid of Yolk-Shell Particles** Luis E. Sanchez Diaz<sup>1</sup>, Magdaleno Medina Noyola<sup>2</sup> and Wei-Ren Chen<sup>1</sup>; <sup>1</sup>Biology and Soft Matter, ORNL, Oak Ridge, Tennessee; <sup>2</sup>Instituto de Fisica UASLP, San Luis Potosi, San Luis Potosi, Mexico.

SESSION D4: Dynamics of Soft Matter  
Session Chair: Souleymane Diallo  
Tuesday Afternoon, June 3, 2014  
Tennessee Ballroom A

**1:45 PM \*D4.01**

**Dynamical Crossover in Soft Colloids Below the Overlap Concentration** Xin Li<sup>1</sup>, Luis E. Sanchez-Diaz<sup>1</sup>, Changwoo Do<sup>1</sup>, Gregory S. Smith<sup>1</sup>, Lionel Porcar<sup>2</sup>, Yun Liu<sup>4,3</sup>, Peter Falus<sup>2</sup>, William A. Hamilton<sup>1</sup>, Takeshi Egami<sup>5,1</sup>, Bin Wu<sup>1</sup> and Wei-Ren Chen<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Institut Laue-Langevin, Grenoble, France; <sup>3</sup>NIST Center for Neutron Research, Gaithersburg, Maryland; <sup>4</sup>University of Delaware, Newark, Delaware; <sup>5</sup>The University of Tennessee, Knoxville, Tennessee.

**2:15 PM D4.02**

**Effects of Acid and Ionic Aggregation on the Polymer Dynamics in Precise Ionomers** Luri R. Middleton<sup>1</sup>, Jacob Tarver<sup>2</sup>, Jenny Kim<sup>2</sup>, Jason Azoulay<sup>3</sup>, Dustin Murtagh<sup>3</sup>, Joseph Cordaro<sup>3</sup>, Madhu Tyagi<sup>2</sup>, Christopher Soles<sup>2</sup> and Karen Winey<sup>1</sup>; <sup>1</sup>Material Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania; <sup>2</sup>Polymers Division Electronics Materials Group, National Institute of Standards and Technology, Gaithersburg, Maryland; <sup>3</sup>Center for Integrated Nanotechnologies, Sandia National Laboratories, Albuquerque, New Mexico.

**2:30 PM D4.03**

**Non-Monotonic Temperature Dependence of the Relaxation Time in Glass-Forming Metallic Liquid** Abhishek Jaiswal<sup>1</sup>, Yang

Zhang<sup>1,2</sup>, Takeshi Egami<sup>3,6</sup>, Konstantin Lokshin<sup>3,6</sup>, Georg Ehlers<sup>4</sup>, Andrey Podlesnyak<sup>4</sup> and Rebecca Mills<sup>5</sup>; <sup>1</sup>Nuclear, Plasma and Radiological Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois; <sup>2</sup>Material Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois; <sup>3</sup>Material Science and Engineering, University of Tennessee, Knoxville, Tennessee; <sup>4</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>5</sup>Instrument and Source Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>6</sup>Joint Institute for Neutron Sciences, University of Tennessee, Knoxville, Tennessee.

## 2:45 PM D4.04

**Excess Wing in Glass-Forming Glycerol and LiCl-Glycerol Mixtures Detected by Neutron Scattering** Sudipta Gupta<sup>1</sup>, Nikolas Arend<sup>2</sup>, Peter Lunkenheimer<sup>3</sup>, Alois Loidl<sup>3</sup>, Laura Stingaciu<sup>1</sup>, Nina Jalarvo<sup>1</sup>, Eugene Mamontov<sup>4</sup> and Michael Ohl<sup>1</sup>; <sup>1</sup>JCNS-SNS Oak Ridge National Laboratory (ORNL), Oak Ridge, Tennessee; <sup>2</sup>Juelich Centre for Neutron Science JCNS, Forschungszentrum Juelich GmbH, Outstation at MLZ, Lichtenbergstrasse 1, 85747 Garching, Germany, Munich, Germany; <sup>3</sup>Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany, Augsburg, Germany; <sup>4</sup>SNS, Neutron Sciences Directorate, Oak Ridge National Laboratory (ORNL), 1 Bethel Valley Road, Oak Ridge, Tennessee.

## 3:00 PM D4.05

**Dynamics of Water in Polyethylene Oxide (PEO) Matrix in the Presence of Li<sup>+</sup> Ions** Zhe Zhang<sup>1</sup>, Kunlun Hong<sup>2</sup>, Niina Julavo<sup>3</sup>, Michael Ohl<sup>3</sup>, Souleymane Omar Diallo<sup>4</sup> and Changwoo Do<sup>1</sup>; <sup>1</sup>Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Juelich Centre for Neutron Science, Juelich, Juelich, Germany; <sup>4</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## 3:15 PM D4.06

**Dynamics of Water in Sulfonated Poly(phenylene) Membranes** Naresh C. Osti<sup>1</sup>, Thusitha N. Etampawala<sup>1</sup>, Umesh M. Shrestha<sup>1</sup>, Souleymane O. Diallo<sup>3</sup>, Christopher J. Cornelius<sup>2</sup> and Dvora Perahia<sup>1</sup>; <sup>1</sup>Department of Chemistry, Clemson University, Clemson, South Carolina; <sup>2</sup>Chemical & Biomolecular Engineering, University of Nebraska-Lincoln, Lincoln, Nebraska; <sup>3</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

SESSION DP3: Poster Session III: Soft Matter  
Tuesday Afternoon, June 3, 2014  
3:30 PM  
Summit II

## DP3.01

**The Effect of Charge on Lamellar Phases, in Oil and Water Rich Environments, Investigated by SANS** Robert Bradbury<sup>1,2</sup> and Michihiro Nagao<sup>1,2</sup>; <sup>1</sup>Center for Exploration of Energy and Matter, Indiana University, Bloomington, Indiana; <sup>2</sup>NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland.

## DP3.02

**Quantifying The Dynamic Heterogeneity Of Glassy Matter From The Relaxation Time Spectrum** Zhikun Cai<sup>1</sup> and Yang Zhang<sup>1,2</sup>; <sup>1</sup>Department of Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois; <sup>2</sup>Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois.

## DP3.03

**Multiscale Structure of Calcium- and Magnesium-Silicate-Hydrate Gels** Wei-Shan Chiang<sup>1</sup>, Giovanni Ferraro<sup>2</sup>, Emiliano Fratini<sup>2</sup>, Francesca Ridi<sup>2</sup>, Yi-Qi Yeh<sup>3</sup>, U-Ser Jeng<sup>3</sup>, Piero Baglioni<sup>2</sup> and Sow-Hsin Chen<sup>1</sup>; <sup>1</sup>Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts; <sup>2</sup>Department of Chemistry "Ugo Schiff" and CSGI, University of Florence, Florence, Italy; <sup>3</sup>National Synchrotron Radiation Research Center, Hsinchu, Taiwan.

## DP3.04

**Investigation of Morphology Change of Opto-Electronic Conjugated Polymers in Block Copolymer/Water Using SANS** Youngkyu Han and Changwoo Do; Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## DP3.05

**Structure Study of Self-Assemblies with Ionic Liquid** Mahn Won Kim<sup>1,2</sup>, Tac Hui Kang<sup>1</sup> and Yoonnam Jeon<sup>1,3</sup>; <sup>1</sup>Korea Advanced Institute of Science and Technology, Daejeon, Korea, Republic of; <sup>2</sup>Gwangju Institute of Science and Technology, Gwangju, Korea, Republic of; <sup>3</sup>Jeonnam Technopark, Jeonnam, Korea, Republic of.

## DP3.06

**Vertical Scan of the Middle, Bicontinuous Microemulsion Phase via SANS Through Use of a New Vertical Stage** Sample Environment Sai V. Pingali<sup>2</sup>, Volker S. Urban<sup>2</sup>, Hugh M. O'Neill<sup>2</sup>, Rachel N. Dunlap<sup>2</sup>, Paul Langan<sup>2</sup>, Douglas G. Hayes<sup>1</sup> and Ran Ye<sup>1</sup>; <sup>1</sup>Biosystems Engineering and Soil Science, University of Tennessee, Knoxville, Tennessee; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## DP3.07

**DNA in Choline-Chloride/Urea Deep Eutectic Solvent** Liel Sapir<sup>1</sup>, Christopher Stanley<sup>2</sup> and Daniel Harries<sup>1</sup>; <sup>1</sup>Institute of Chemistry and the Fritz Haber Center, The Hebrew University of Jerusalem, Jerusalem, Israel; <sup>2</sup>Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

SESSION DP4: Poster Session IV: Soft Matter  
Wednesday Evening, June 4, 2014  
5:30 PM  
Summit II

## DP4.01

**Lack of Pore Defects in Vesicles of Binary Lipid Mixtures Above T<sub>m</sub>** Paul Butler<sup>1</sup>, Andreea Woodka<sup>3</sup> and Lionel Porcar<sup>2</sup>; <sup>1</sup>NIST, Gaithersburg, Maryland; <sup>2</sup>ILL, Grenoble, France; <sup>3</sup>United States Military Academy, West Point, New York.

## DP4.02

**Bilayer Self Assembly on a Hydrophilic, Deterministically Nanopatterned Surface** Gregory Smith<sup>1</sup>, Seung-Yong Jung<sup>2</sup>, James Browning<sup>3</sup>, Jong Keum<sup>3</sup>, Nikolay Lavrik<sup>4</sup>, Mussie Alemseghed<sup>3,5</sup> and Pat Collier<sup>4</sup>; <sup>1</sup>Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Gladstone Institute, University of California San Francisco, San Francisco, California; <sup>3</sup>Chemical and Engineering Materials Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>5</sup>Department of Chemical and Materials Engineering, University of Cincinnati, Cincinnati, Ohio.

## DP4.03

**SANS Analysis of Lipase-Catalyzed Biodiesel Synthesis in Water-in-Oil Microemulsions** Douglas G. Hayes<sup>1</sup>, Ran Ye<sup>1</sup>, Volker S. Urban<sup>2</sup> and Sai V. Pingali<sup>2</sup>; <sup>1</sup>Biosystems Engineering and Soil Science, University of Tennessee, Knoxville, Tennessee; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## DP4.04

**Structural Study of MonoPEGylated Human Parathyroid Hormone Fragments hPTH(1-34) in Solution Revealed by Small-Angle Neutron and X-Ray Scattering** Chih-Ying Liu<sup>1</sup>, Hsiu-Yun Lai<sup>2</sup>, Xin Li<sup>3</sup>, Wen-Yi Chen<sup>1</sup> and E-Wen Huang<sup>1</sup>; <sup>1</sup>Department of Chemical and Materials Engineering, National Central University, Jhongli, Taiwan; <sup>2</sup>Department of Family Medicine, National Taiwan University Hospital, Hsinchu, Taiwan; <sup>3</sup>Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## DP4.05

**Conducting Polymer Nanostructures and Nanocomposites: Hierarchical Assembly via Molecular Electrochemistry and Property Characterization** C. Price, H. Heyworth and Sanju Gupta; Physics and Astronomy, Western Kentucky University, Bowling Green, Kentucky.

## DP4.06

**Dynamic Light Scattering of Imprinted NIPAm Gels** Charlezetta E. Stokes and Kimani A. Stancil; Physics, Howard University, Washington, District of Columbia.

## DP4.07

**Scattering Theory for Branched and Tortuous Persistent Chains** Karsten Vogt and Gregory Beaucage; University of Cincinnati, Cincinnati, Ohio.

## DP4.08

**Nucleation Pathways of CO<sub>2</sub> Condensation under Mesoporous**

SESSION D5: Colloidal and Self-Assembled Systems  
Session Chair: Gregory Smith  
Thursday Morning, June 5, 2014  
Tennessee Ballroom A

**9:45 AM \*D5.01**

**Building and Breaking Large-Scale Structure in Nanoemulsion Colloidal Gels** Matthew E. Helgeson<sup>1</sup>, Juntae

Kim<sup>1</sup>, Yongxiang Gao<sup>1</sup> and Dimitri Merger<sup>1,2</sup>; <sup>1</sup>Chemical Engineering, UC Santa Barbara, Santa Barbara, California;

<sup>2</sup>Karlsruhe Institute of Technology, Karlsruhe, Germany.

**10:15 AM \*D5.02**

**Solution Phase Structures of Supramolecular Architectures**

Jerry L. Atwood<sup>1</sup>, Harshita Kumari<sup>1</sup> and Steven R. Kline<sup>2</sup>;

<sup>1</sup>Department of Chemistry, University of Missouri-Columbia, Columbia, Missouri; <sup>2</sup>Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland.

**10:45 AM D5.03**

**Hierarchical Self-Assemblies of 1D Nanoparticles in Amphiphilic Molecular Systems** Sung-Min Choi<sup>1</sup>, Sung-Hwan

Lim<sup>1</sup>, Hyung-Sik Jang<sup>1</sup>, Jac-Min Ha<sup>1</sup>, Tae-Hwan Kim<sup>2</sup>, Pawel Kwansnieski<sup>3</sup> and Theyencheri Narayanan<sup>3</sup>; <sup>1</sup>Department of Nuclear and Quantum Engineering, KAIST, Daejeon, Korea, Republic of;

<sup>2</sup>HANARO Neutron Science Division, KAERI, Daejeon, Korea, Republic of; <sup>3</sup>European Synchrotron Radiation Facility, Grenoble, France.

**11:00 AM D5.04**

**Understanding a New Sustainable Technology for Water Purification Using Small-Angle Scattering and Reflection**

Adrian R. Rennie<sup>1</sup>, Maja S. Hellsing<sup>1</sup>, Habbauka M. Kwaambwa<sup>2</sup>, Bonang Nkoane<sup>3</sup> and Fiona Nermark<sup>3</sup>; <sup>1</sup>Dept. of Physics & Astronomy, Uppsala University, Uppsala, Sweden; <sup>2</sup>School of Health

& Life Sciences, Polytechnic of Namibia, Windhoek, Namibia; <sup>3</sup>Department of Chemistry, University of Botswana, Gaborone, Botswana.

**11:15 AM D5.05**

**SANS Analysis of Proteins Encapsulated into Bicontinuous Microemulsions Phase of Winsor-III Systems**

Douglas G. Hayes<sup>1</sup>, Ran Ye<sup>1</sup>, Volker S. Urban<sup>2</sup>, Sai V. Pingali<sup>2</sup>, Hugh

M. O'Neill<sup>2</sup>, Rachel N. Dunlap<sup>2</sup> and Paul Langan<sup>2</sup>; <sup>1</sup>Biosystems Engineering and Soil Science, University of Tennessee, Knoxville, Tennessee; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee.

**11:30 AM D5.06**

**Scattering Function of Star Polymer with Excluded Volume Effect** Xin Li<sup>1</sup>, Lionel Porcar<sup>3</sup>, Yun Liu<sup>4,2</sup>, Changwoo Do<sup>1</sup>, Gregory

S. Smith<sup>1</sup> and Wei-Ren Chen<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>NIST Center for Neutron Research, Gaithersburg, Maryland; <sup>3</sup>Institut Laue-Langevin, Grenoble, France; <sup>4</sup>University of Delaware, Newark, Delaware.

\* Invited paper

SESSION EP1: Poster Session I: Biology  
Sunday Evening, June 1, 2014  
5:00 PM  
Summit II

## EP1.01

**Investigation of the Coupled Folding and Binding of Alpha-Synuclein in Lipid Membranes by Small Angle Neutron Scattering** Divina Anunciado, Shuo Qian and Hugh O'Neill; Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## EP1.02

**Investigation of Natural Bombyx Mori Silk Fibroin Proteins Using INS** Christopher A. Crain<sup>1</sup>, Nicholas Strange<sup>1</sup>, Luke L.

Daemen<sup>2</sup>, Monika Hartl<sup>2</sup>, Souleymane O. Diallo<sup>3</sup> and John Z. Larese<sup>1</sup>; <sup>1</sup>Chemistry, University of Tennessee, Knoxville, Tennessee; <sup>2</sup>Lujan Center, LANL, Knoxville, New Mexico; <sup>3</sup>Spallation Neutron Source, ORNL, Oak Ridge, Tennessee.

## EP1.03

**Functional and Structural Characterization of the Enzybiotic PlyC at Lipid Membrane** Frank Heinrich<sup>1,2</sup>, Marilia Cabral Do Rego Barros<sup>1</sup>, Tarek Vennemann<sup>1</sup>, Daniel C.

Nelson<sup>3</sup> and Mathias Losche<sup>1,2,4</sup>; <sup>1</sup>Department of Physics, Carnegie Mellon, Pittsburgh, Pennsylvania; <sup>2</sup>NIST Center for Neutron Research (NCNR), Gaithersburg, Maryland; <sup>3</sup>Institute for Bioscience and Biotechnology, University of Maryland, Rockville, Maryland; <sup>4</sup>Department of Biomedical Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania.

## EP1.04

**A Second Allosteric Switch in Periplasmic Binding Protein Mediated ABC Transport** Sudipa Ghimire-Rijal, Xun Lu, Christopher Stanley, Dean Myles and Matthew Cuneo; Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## EP1.05

**Digestion of Amorphous Cellulose Films by Endoglucanases: Effect of the Cellulose Binding Module** Vimalier Reyes-Ortiz<sup>1,4</sup>, Candice Halbert<sup>3</sup>, Richard A. Heins<sup>1,2</sup>, Kenneth L. Sale<sup>1,2</sup>, Blake A. Simmons<sup>1,2</sup>, Danielle Tullman-Ercek<sup>4</sup> and Michael S. Kent<sup>1,5</sup>; <sup>1</sup>Joint BioEnergy Institute, Emeryville, California; <sup>2</sup>Sandia National Labs, Livermore, California; <sup>3</sup>Oak Ridge National Lab, Oak Ridge, Tennessee; <sup>4</sup>University of California, Berkeley, California; <sup>5</sup>Sandia National Labs, Albuquerque, New Mexico.

## EP1.06

**SANS Study of Moisture-Induced Changes in the Cell Wall of Loblolly Pine** Nayomi Plaza<sup>1,2</sup>, Shuo Qian<sup>4</sup>, William Heller<sup>3</sup>, Sai V. Pingali<sup>4</sup> and Joseph Jakes<sup>2</sup>; <sup>1</sup>Materials Science Program, University of Wisconsin Madison, Madison, Wisconsin; <sup>2</sup>Forest Biopolymers Science and Engineering, USDA Forest Service, Forest Products Laboratory, Madison, Wisconsin; <sup>3</sup>Center for Structural Molecular Biology Biology and Soft Matter Division, Oak Ridge National Laboratory, Madison, Tennessee; <sup>4</sup>Biology and Soft Matter Division Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## EP1.07

**Dynamics of a Large Oligomeric Protein Under High Pressure Studied by Neutron Scattering** Utsab R. Shrestha<sup>1</sup>, Kurt W. Van Delinder<sup>1</sup>, Manavalan Gajapathy<sup>2</sup>, John Copley<sup>3</sup>, Juscelino Leao<sup>3</sup>, Joseph Ng<sup>2</sup> and Xiang-Qiang Chu<sup>1</sup>; <sup>1</sup>Department of Physics and Astronomy, Wayne State University, Detroit, Michigan; <sup>2</sup>Department of Biological Sciences, University of Alabama in Huntsville, Huntsville, Alabama; <sup>3</sup>NIST Center for Neutron Research, NIST, Gaithersburg, Maryland.

## EP1.08

**The Bio-Deuteration Lab at Oak Ridge National Laboratory** Kevin Weiss, Qiu Zhang, Hugh O'Neill, Volker Urban and Paul Langan; Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## EP1.09

**Internal Dynamics of Immunoglobulin G - Influence of Blocking Agent** Laura R. Stingaciu<sup>1,3</sup>, Ralf Biehl<sup>2</sup>, Andreas Stadler<sup>2</sup>, Changwoo Do<sup>3</sup>, Oxana Ivanova<sup>4</sup>, Noemi Szekeley<sup>4</sup> and Michael Ohl<sup>1,3</sup>; <sup>1</sup>JCN-SNS, Forschungszentrum Juelich GmbH, Juelich, Germany; <sup>2</sup>ICSI, Forschungszentrum Juelich GmbH, Juelich, Germany; <sup>3</sup>NScD, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>JCN-S1-FRM11, Forschungszentrum Juelich GmbH,

SESSION E1: Protein Structures and Dynamics I  
Session Chair: Shuo Qian  
Monday Afternoon, June 2, 2014  
Tennessee Ballroom B

## 4:00 PM \*E1.01

**Ultra-High Resolution Protein Crystallography: Neutron Structure of Crambin at 1.1 Å** Julian Chen<sup>1,2</sup>, Bryant L. Hanson<sup>2</sup>, S. Z. Fisher<sup>1</sup>, Paul Langan<sup>2,3</sup> and Andrey Kovelevsky<sup>3</sup>; <sup>1</sup>Bioscience Division, Los Alamos National Laboratory, Los Alamos, New Mexico; <sup>2</sup>Department of Chemistry, University of Toledo, Toledo, Ohio; <sup>3</sup>Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## 4:30 PM E1.02

**Structural Models Of Gelsolin: Actin Binary and Ternary Complexes Constrained by Small-Angle Scattering Data** Joanna K. Krueger<sup>1</sup>, Ryan C. Oliver<sup>2,1</sup>, Amin Sagar<sup>3</sup>, Fnu Ashish<sup>3,1</sup>, Nagesh Peddada<sup>3</sup>, Vikas Choudhary<sup>3</sup>, Yawar Mir<sup>3</sup> and Renu Garg<sup>3</sup>; <sup>1</sup>Chemistry, UNC Charlotte, Charlotte, North Carolina; <sup>2</sup>Chemistry, University of Virginia, Charlottesville, Virginia; <sup>3</sup>CSIR-Institute of Microbial Technology, Chandigarh, India.

## 4:45 PM E1.03

**Important Dynamics of Catalytic Subunit of Protein Kinase A: A Case Study of Combined Molecular Dynamics Simulations and Small Angle Neutron Scattering** Jianhui Tian<sup>1</sup>, Amit Das<sup>1</sup>, Oksana Gerlits<sup>1</sup>, Andrii Kovalevsky<sup>1</sup>, Paul Langan<sup>1</sup>, Loukas Petridis<sup>2</sup> and William T. Heller<sup>1</sup>; <sup>1</sup>Biology and Soft Matter Division, Oak Ridge National Lab, Oak Ridge, Tennessee; <sup>2</sup>Center for Molecular Biophysics, Oak Ridge National Lab, Oak Ridge, Tennessee.

## 5:00 PM E1.04

**Conformational Sub-States and Solvent Driven Protein Dynamics Impacts Enzyme Catalysis** Jose Borreguero<sup>1</sup>, Matthew Cuneo<sup>2</sup>, Arvind Ramanathan<sup>3</sup>, Junhong He<sup>2</sup>, Michael R. Duff<sup>4</sup>, Chakra Chennubhotla<sup>5</sup>, Flora Meilleur<sup>2,6</sup>, Elizabeth E. Howell<sup>4</sup>, Kenneth Herwig<sup>7</sup>, Dean A. Myles<sup>2</sup> and Pratul K. Agarwal<sup>3</sup>; <sup>1</sup>Neutron Data & Visualization Division, ORNL/UT-Batelle, Oak Ridge, Tennessee; <sup>2</sup>Biology & Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Department of Biochemistry and Cellular and Molecular Biology, University of Tennessee, Knoxville, Tennessee; <sup>5</sup>Department of Computational and Systems Biology, School of Medicine, University of Pittsburgh, Pittsburgh, Pennsylvania; <sup>6</sup>Molecular and Structural Biochemistry Department, North Carolina State University, Raleigh, North Carolina; <sup>7</sup>Instrument and Source Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## 5:15 PM E1.05

**De Gennes Narrowing Describes the Relative Motion of Protein Domains** Liang Hong and Jeremy C. Smith; Center for Molecular Biophysics, Oak Ridge, Tennessee.

SESSION EP2: Poster Session II: Biology  
Monday Evening, June 2, 2014  
5:30 PM  
Summit II

## EP2.01

**Behavior of Lipids supported on Silica Nanoparticles** Li Ge<sup>1</sup>, Ursula Perez-Salas<sup>1</sup>, Jeffrey M. Breidigan<sup>1</sup> and Lionel Porcar<sup>2</sup>; <sup>1</sup>University of Illinois at Chicago, Oak Forest, Illinois; <sup>2</sup>Institut Laue-Langevin, Grenoble, France.

## EP2.02

**Dynamics of Hydrated tRNA on Nanodiamond Surface Studied by Quasi-Elastic Neutron Scattering** Gurpreet K. Dhindsa<sup>1</sup>, Vadym Mochalin<sup>2</sup>, Hugh O'Neill<sup>3</sup>, Yuri Gogotsi<sup>2</sup>, Xiang Qiang Chu<sup>1</sup> and Panchapakesan Ganesh<sup>4</sup>; <sup>1</sup>Wayne State University, Detroit, Michigan; <sup>2</sup>Drexel University, Philadelphia, Pennsylvania; <sup>3</sup>Biology and Soft Matter, Oakridge, Tennessee; <sup>4</sup>Center for Nanophase Materials Sciences, oakridge, Tennessee.

## EP2.03

**Production and Characterization of Deuterated Switchgrass and Annual Grasses for Neutron Studies** Barbara R. Evans<sup>1</sup>, Garima Bali<sup>2</sup>, Riddhi Shah<sup>3</sup>, Artthtur J. Ragauskas<sup>2</sup>, Hugh M. O'Neill<sup>3</sup>, Sai V. Pingali<sup>3</sup>, Daisuke Sawada<sup>3</sup>, Volker Urban<sup>3</sup>, Paul A.

Langan<sup>3</sup> and Brian H. Davison<sup>4</sup>; <sup>1</sup>Chemical Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Institute of Paper Science and Technology, Georgia Institute of Technology, Atlanta, Georgia; <sup>3</sup>Biology and Soft Matter, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### **EP2.04**

**Extracting Q Independent Motional Displacements in Proteins from Experiment** Henry Glyde and Derya Vural; Physics, University of Delaware, Newark, Delaware.

#### **EP2.05**

**Myristoylation Restricts Orientation of GRASP on Membranes and is Critical for Membrane Tethering** Frank Heinrich<sup>1,2</sup>, Hirsh Nanda<sup>1,2</sup>, Haw Zan Goh<sup>1,3</sup>, Colin Bachert<sup>4</sup>, Adam D. Linstedt<sup>4</sup> and Mathias Loesche<sup>1,2,5</sup>; <sup>1</sup>Department of Physics, Carnegie Mellon, Pittsburgh, Pennsylvania; <sup>2</sup>NIST Center for Neutron Research (NCNR), Gaithersburg, Maryland; <sup>3</sup>School of Materials Science and Engineering, Nanyang Technological University, Singapore, Singapore; <sup>4</sup>Department of Biological Sciences, Carnegie Mellon University, Pittsburgh, Pennsylvania; <sup>5</sup>Department of Biomedical Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania.

#### **EP2.06**

**Toward a Unified View of the Structure and Dynamics of Water Associated with Single-Supported Zwitterionic and Anionic Membranes** [1] Andrew Miskowiec<sup>1</sup>, Zachary Buck<sup>1</sup>, Helmut Kaiser<sup>1</sup>, Haskell Taub<sup>1</sup>, Flemming Y. Hansen<sup>2,1</sup>, Madhusudan Tyagi<sup>3</sup>, Souleymane Diallo<sup>4</sup>, Eugene Mamontov<sup>4</sup> and Kenneth Herwig<sup>4</sup>; <sup>1</sup>Physics and Astronomy, University of Missouri, Columbia, Missouri; <sup>2</sup>Department of Chemistry, Technical University of Denmark, Lyngby, Denmark; <sup>3</sup>Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland; <sup>4</sup>Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### **EP2.07**

**Elastic Neutron Diffraction from Water Associated with Zwitterionic and Anionic Single-Supported Membranes** [1] Zachary Buck<sup>1</sup>, Andrew Miskowiec<sup>1</sup>, Helmut Kaiser<sup>1</sup>, Flemming Y. Hansen<sup>2,1</sup> and Haskell Taub<sup>1</sup>; <sup>1</sup>Physics & Astronomy, University of Missouri, Columbia, Missouri; <sup>2</sup>Chemistry, Technical University of Denmark, Lyngby, Denmark.

#### **EP2.08**

**Bio-SANS, A Neutron Toolbox for Biomacromolecular Studies** Shuo Qian, Sai Venkatesh Pingali, Katherine Bailey, Qiu Zhang, Hugh O'Neill, Kevin Weiss, Volker Urban and Paul Langan; Oak Ridge National Laboratory, Oak Ridge, Tennessee.

SESSION E2: Lipids  
Session Chair: Andrew Miskowiec  
Tuesday Morning, June 3, 2014  
Tennessee Ballroom B

#### **10:15 AM \*E2.01**

**Self-Assembled Lipid-Based Nanodiscs, Their Characterizations, and Applications** Mu-Ping Nieh, <sup>1</sup>Institute of Materials Science, University of Connecticut, Storrs, Connecticut; <sup>2</sup>Department of Chemical & Biomolecular Engineering, University of Connecticut, Storrs, Connecticut; <sup>3</sup>Department of Biomedical Engineering, University of Connecticut, Storrs, Connecticut.

#### **10:45 AM E2.02**

**Alpha-Tocopherol in Model Membranes: A Structure-Function Relationship** Drew Marquardt<sup>1</sup>, Justin A. Williams<sup>2</sup>, Norbert Kucerka<sup>3</sup>, Jeffrey Atkinson<sup>1</sup>, Stephen R. Wassall<sup>2</sup>, John Katsaras<sup>4,1</sup> and Thad A. Harroun<sup>1</sup>; <sup>1</sup>Physics, Brock University, St. Catharines, Ontario, Canada; <sup>2</sup>Physics, Indiana University-Purdue University, Indianapolis, Indiana; <sup>3</sup>Canadian Neutron Beam Centre, National Research Council of Canada, Chalk River, Ontario, Canada; <sup>4</sup>Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### **11:00 AM E2.03**

**Phase Behavior and Composition as a Function of Temperature in DPPC:DLPC Model Membranes with Varying Amounts of Cholesterol** Natalie Krzyzanowski<sup>1</sup>, Sumit Garg<sup>4,1</sup>, Lionel Porcar<sup>2</sup>, Paul D. Butler<sup>3</sup> and Ursula Perez-Salas<sup>1</sup>; <sup>1</sup>Physics, University of Illinois at Chicago, Chicago, Illinois; <sup>2</sup>Large Scale Structures Group, Institut Max von Laue - Paul Langevin, Grenoble, France; <sup>3</sup>Center for Neutron Research, NIST, Gaithersburg, Maryland; <sup>4</sup>Biomaterials, Argonne National Laboratory, Argonne,

Illinois.

#### **11:15 AM E2.04**

**Lateral and Trans-Membrane Diffusion in Membranes: A Two-Dimensional Diffusion Map** Laura Toppozini<sup>1</sup>, Victoria Garcia-Sakai<sup>2</sup> and Maikel Rheinstadter<sup>1</sup>; <sup>1</sup>Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada; <sup>2</sup>ISIS, Rutherford Appleton Laboratory, Didcot, United Kingdom.

#### **11:30 AM E2.05**

**Aspirin Reorganizes the Lipid Membrane** Richard Alsop<sup>1</sup>, Laura Toppozini<sup>1</sup>, Norbert Kucerka<sup>2</sup> and Maikel Rheinstadter<sup>1,2</sup>; <sup>1</sup>McMaster University, Hamilton, Ontario, Canada; <sup>2</sup>Canadian Neutron Beam Centre, Chalk River, Ontario, Canada.

#### **11:45 AM E2.06**

**Lipid-Cholesterol Interactions on the Atomic Scale: Insights into Membrane Formation from Solution** Richard J. Gillams, Sebastian Busch and Sylvia E. McLain; Biochemistry, University of Oxford, Oxford, United Kingdom.

#### **12:00 PM E2.07**

**Steps Towards Developing a Realistic Model of the Gram Negative Bacterial Outer Membrane** Stephen A. Holt<sup>1</sup>, Anton Le Brun<sup>1</sup>, Luke Clifton<sup>2</sup> and Jeremy Lakey<sup>3</sup>; <sup>1</sup>Bragg Institute, ANSTO, Kirrawee DC, New South Wales, Australia; <sup>2</sup>ISIS, Rutherford Appleton Laboratory, Didcot, Oxfordshire, United Kingdom; <sup>3</sup>Institute for Cell and Molecular Biosciences, The University of Newcastle, Newcastle upon Tyne, Tyne and Wear, United Kingdom.

SESSION E3: Proteins Structure and Dynamics II  
Session Chair: Bryan Holland  
Tuesday Afternoon, June 3, 2014  
Tennessee Ballroom B

#### **1:45 PM \*E3.01**

**Secondary Structure and Nanomechanical Properties of Proteins** Jonathan D. Nickels, <sup>1</sup>Joint Institute for Neutron Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Department of Physics, University of Tennessee, Knoxville, Knoxville, Tennessee.

#### **2:15 PM E3.02**

**Accounting for Multiple Species in the Time-Resolved SANS on Huntingtin Aggregation** Christopher Stanley<sup>1</sup>, Tatiana Perevozchikova<sup>2</sup>, Helen McWilliams-Koeppen<sup>2</sup>, Erica Rowe<sup>2</sup> and Valerie Bertheliet<sup>2</sup>; <sup>1</sup>Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Graduate School of Medicine, University of Tennessee Health Science Center, Knoxville, Tennessee.

#### **2:30 PM E3.03**

**Long-Time Intrinsic Mean Square Displacements in Proteins** Henry Glyde<sup>1</sup>, Derya Vural<sup>1</sup>, Liang Hong<sup>2</sup> and Jeremy C. Smith<sup>2</sup>; <sup>1</sup>Physics, University of Delaware, Newark, Delaware; <sup>2</sup>UT/ORNL Center for Molecular Biophysics, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### **2:45 PM E3.04**

**Using Neutron Scattering to Understand the Dynamics and Microrheology of Concentrated Protein Solutions** Paul D. Godfrin<sup>1</sup>, Steven D. Hudson<sup>2</sup>, Kunlun Hong<sup>3</sup>, Peter Falus<sup>4</sup>, Norman J. Wagner<sup>1</sup> and Yun Liu<sup>1,5</sup>; <sup>1</sup>Chemical and Biomolecular Engineering, University of Delaware, Newark, Delaware; <sup>2</sup>Materials Measurement Laboratory, NIST, Gaithersburg, Maryland; <sup>3</sup>Center for Nanophase Materials and Sciences, ORNL, Oak Ridge, Tennessee; <sup>4</sup>Time of Flight and High Resolution Group, ILL, Grenoble, France; <sup>5</sup>Center for Neutron Science, NIST, Gaithersburg, Maryland.

#### **3:00 PM E3.05**

**Water's Role in Aggregation and Conformation for Biomolecules in Solution: Probing the Physics of Life in Solution** Sylvia McLain, Biochemistry, University of Oxford, Oxford, United Kingdom.

#### **3:15 PM E3.06**

**SIMtoEXP 2.0: Software for Comparing Simulations to Experimental Scattering Data** Bryan W. Holland<sup>1</sup>, Norbert Kucerka<sup>2</sup> and D. P. Tieleman<sup>1</sup>; <sup>1</sup>Biological Sciences, University of Calgary, Calgary, Alberta, Canada; <sup>2</sup>Canadian Neutron Beam Centre, National Research Council Canada, Chalk River, Ontario, Canada.

**EP3.01**

**Hierarchical, Self-Similar Structure in Native Squid Pen**  
Fei-Chi Yang, Robert Peters, Hannah Dies, Maikel C. Rheinstadter;  
Department of Physics and Astronomy, McMaster University,  
Hamilton, Ontario, Canada.

**EP3.02**

**Electric Field Studies of Water Mobility in Inorganic and Biological Compounds** Souleymane Diallo, Pelagie Favi, Eugene Mamontov and Hugh O'Neill; Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

**EP3.03**

**Comparison of Solute Profile of Trehalose and Sucrose Between Lamellar Stacks of Dioleoylphosphatidylcholine by Neutron Membrane Diffraction** Christopher J. Garvey<sup>1</sup>, Ben Kent<sup>2</sup>, Taavi Hunt<sup>3</sup>, Bruno Deme<sup>4</sup>, Thomas Hauss<sup>2</sup> and Gary Bryant<sup>3</sup>; <sup>1</sup>ANSTO, Kirrawee DC, New South Wales, Australia; <sup>2</sup>Helmholtz-Zentrum Berlin fuer Materialien und Energie GmbH, Berlin, Germany; <sup>3</sup>Centre for Molecular and Nanoscale Physics, School of Applied Sciences, RMIT University, Melbourne, New South Wales, Australia; <sup>4</sup>Institute Laue-Langevin, Grenoble, France.

**EP3.04**

**Scattering Study of Reversible Cluster Formation in Concentrated Monoclonal Antibody Formulations** Paul D. Godfrin<sup>1</sup>, Steven D. Hudson<sup>2</sup>, Isidro E. Zarraga<sup>3</sup>, Kunlun Hong<sup>4</sup>, Lionel Porcar<sup>5</sup>, Peter Falus<sup>6</sup>, Norman J. Wagner<sup>1</sup> and Yun Liu<sup>7</sup>; <sup>1</sup>Chemical and Biomolecular Engineering, University of Delaware, Newark, Delaware; <sup>2</sup>Materials Measurement Laboratory, NIST, Gaithersburg, Maryland; <sup>3</sup>Late Stage Pharmaceutical Development, Genentech Inc., South San Francisco, California; <sup>4</sup>Center for Nanophase Materials and Sciences, ORNL, Oak Ridge, Tennessee; <sup>5</sup>Large Scale Structures, ILL, Grenoble, France; <sup>6</sup>Time of Flight and High Resolution Group, ILL, Grenoble, France; <sup>7</sup>Center for Neutron Science, NIST, Gaithersburg, Maryland.

**EP3.05**

**Endothelial Interfaces – Master Gatekeepers of the Cardiovascular System** Ann Junghans<sup>1</sup>, Luka Pocivavsek<sup>2</sup>, Konstantin Birukov<sup>3</sup>, Mary Jo Waltman<sup>1</sup> and Jaroslaw Majewski<sup>1</sup>; <sup>1</sup>Lujan Center, LANL, Los Alamos, New Mexico; <sup>2</sup>Department of Surgery, University of Pittsburgh Medical Center, Pittsburgh, Pennsylvania; <sup>3</sup>Department of Medicine, University of Chicago, Chicago, Illinois.

**EP3.06**

**Contrast Variation to Determine Detergent-Lipid Organization and Structural Transitions Between Bicelle and Mixed Micelle Conditions** Ryan Oliver<sup>1</sup>, Joanna Krueger<sup>2</sup> and Linda Columbus<sup>1</sup>; <sup>1</sup>Chemistry, Univ of Virginia, Charlottesville, Virginia; <sup>2</sup>Chemistry, Univ of N Carolina at Charlotte, Charlotte, North Carolina.

**EP3.07**

**Structural Investigations of Xylan-Cellulose Composites** Riddhi S. Shah<sup>1</sup>, Daisuke Sawada<sup>1</sup>, Hugh M. O'Neill<sup>1</sup>, Sai Venkatesh Pingali<sup>1</sup>, Barbara R. Evans<sup>1</sup>, Garima Bali<sup>2</sup>, Arthur Ragauskas<sup>2</sup>, Volker Urban<sup>1</sup>, Paul A. Langan<sup>1</sup> and Brian H. Davison<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Georgia Institute of Technology, Atlanta, Georgia.

**EP3.08**

**Structural Studies on Plant Cellulose Synthase** Venu Gopal Vandavasi<sup>1</sup>, William Heller<sup>1</sup>, Loukas Petridis<sup>2</sup>, Udaya Kalluri<sup>3</sup>, Leighton Coates<sup>1</sup>, Jeremy Smith<sup>2</sup>, Benjamin Linder<sup>2</sup>, Jens Meiler<sup>4</sup> and Hugh O'Neill<sup>1</sup>; <sup>1</sup>Biology & Soft Matter Division, ORNL, Oak Ridge, Tennessee; <sup>2</sup>Center for Computational Biophysics, ORNL, Oak Ridge, Tennessee; <sup>3</sup>Bio Sciences Division, ORNL, Oak Ridge, Tennessee; <sup>4</sup>Department of Chemistry, Vanderbilt University, Nashville, Tennessee.

**10:15 AM \*E4.01**

**Joining Neutron Scattering and Simulations for Complex Biological Membranes** Xiaolin Cheng<sup>1</sup>, Jianjun Pan<sup>2</sup>, Jonathan Nickels<sup>1</sup>, Frederick A. Heberle<sup>1</sup> and John Katsaras<sup>1</sup>; <sup>1</sup>ORNL, Oak Ridge, Tennessee; <sup>2</sup>Department of Physics, University of South Florida, Tampa, Florida.

**10:45 AM E4.02**

**Ultra Small Angle Neutron Scattering Studies of Actively Metabolising Red Blood Cells of Different Shapes and Sizes** Christopher J. Garvey<sup>1</sup> and Philip W. Kuchel<sup>2</sup>; <sup>1</sup>ANSTO, Kirrawee DC, New South Wales, Australia; <sup>2</sup>School of Molecular Bioscience, University of Sydney, New South Wales, Australia.

**11:00 AM E4.03**

**Small-Angle Neutron Scattering Techniques for Probing Lateral Organization of Lipid Membranes in Live Cells** Frederick A. Heberle<sup>1</sup>, Jonathan D. Nickels<sup>1</sup>, Sneha Chatterjee<sup>2</sup>, John Katsaras<sup>1</sup>, Robert R. Standaert<sup>1,2</sup>, Dean A. Myles<sup>1</sup> and James G. Elkins<sup>2</sup>; <sup>1</sup>Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

**11:15 AM E4.04**

**Molecular Adaptation of Deep Sea Organisms to Extreme Conditions** Nicolas Martinez<sup>1,2,3</sup>, Gregoire Michoud<sup>4</sup>, Anais Cario<sup>5</sup>, Mohamed Jebbar<sup>4</sup>, Philippe Oger<sup>5</sup>, Bruno Franzetti<sup>3</sup> and Judith Peters<sup>1,2,3</sup>; <sup>1</sup>Universite Joseph Fourier, Grenoble, France; <sup>2</sup>Institut Laue Langevin, Grenoble, France; <sup>3</sup>Institut de Biologie Structurale, Grenoble, France; <sup>4</sup>Laboratoire de Microbiologie des Conditions Extremes, Plouzané, France; <sup>5</sup>Laboratoire de Geologie de Lyon, Lyon, France.

**11:30 AM E4.05**

**Neutron Spin Echo on a Living Cell: The Dynamics of Cyanobacterial Thylakoid Membrane** Laura R. Stingaciu<sup>1,2</sup>, Hugh O'Neill<sup>2</sup>, Michelle Liberton<sup>3</sup>, Volker Urban<sup>2</sup>, Himadri Pakrasi<sup>3</sup> and Michael Ohl<sup>1,2</sup>; <sup>1</sup>JCNS1-SNS, Forschungszentrum Juelich GmbH, Juelich, Germany; <sup>2</sup>NScD, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Department of Biology, Washington University St. Louis, St. Louis, Missouri.

**11:45 AM E4.06**

**SANS Reveals Thylakoid Membrane Ultrastructural Changes During Photosynthesis In-Vivo** Renata Ummcp<sup>1,2</sup>, Gergely Nagy<sup>1,2</sup> and Gyoza Garab<sup>3</sup>; <sup>1</sup>Paul Scherrer Institution, Villigen, Switzerland; <sup>2</sup>Wigner Research Center SZFI, Budapest, Hungary; <sup>3</sup>Biological Research Center, Szeged, Hungary.

**4:00 PM \*E5.01**

**Structure and Function of Membrane Proteins in Bio-Mimetic Lipid Environments: Insights from Neutron Reflectivity and MD Simulations** David Hoogerheide<sup>1</sup>, Dan Scott<sup>1</sup>, Frank Heinrich<sup>1,2</sup>, Mathias Loesche<sup>1,2,3</sup> and Hirsh Nanda<sup>1,2</sup>; <sup>1</sup>NIST Center for Neutron Research (NCNR), Gaithersburg, Maryland; <sup>2</sup>Department of Physics, Carnegie Mellon University, Pittsburgh, Pennsylvania; <sup>3</sup>Department of Biomedical Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania.

**4:30 PM E5.02**

**Studying the Effect of Protein-Detergent Interactions on the Solution Structure of Photosystem I (PSI) from Thermosynechococcus Elongatus** Rosemary Le<sup>1</sup>, Bradley J. Harris<sup>1</sup>, Ifeyinwa J. Iwuchukwu<sup>1</sup>, Barry D. Bruce<sup>2</sup>, Xiaolin Cheng<sup>3</sup>, Shuo Qian<sup>4</sup>, William T. Heller<sup>4</sup>, Hugh O'Neill<sup>4</sup> and Paul D. Frymier<sup>1</sup>; <sup>1</sup>Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, Tennessee; <sup>2</sup>Biochemistry and Cellular and Molecular Biology, University of Tennessee, Knoxville, Tennessee; <sup>3</sup>Center for Molecular Biophysics, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

4:45 PM **E5.03**

**Molecular Details of the Association of  $\alpha$ -Synuclein with Lipid Membranes** Zhiping Jiang<sup>3</sup>, Frank Heinrich<sup>1,2</sup>, Ryan P. McGlinchey<sup>3</sup>, Sara K. Hess<sup>3</sup>, Thai L. Yap<sup>3</sup>, Ellen Sidransky<sup>4</sup> and Jennifer C. Lee<sup>3</sup>; <sup>1</sup>Department of Physics, Carnegie Mellon, Pittsburgh, Pennsylvania; <sup>2</sup>Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland; <sup>3</sup>National Heart, Lung, and Blood Institute, National Institute of Health, Bethesda, Maryland; <sup>4</sup>National Human Genome Research Institute, National Institute of Health, Bethesda, Maryland.

5:00 PM **E5.04**

**Combining Neutron Reflectivity and Hydrogen Deuterium Exchange Mass Spectrometry to Resolve Structural Details of Membrane Associated Proteins** Gregory P. Pirrone<sup>3</sup>, Bulent Akgun<sup>4</sup>, Xiaomeng Shi<sup>3</sup>, Hirsh Nanda<sup>2</sup>, Sushil Satija<sup>2</sup>, John R. Engen<sup>3</sup> and Michael S. Kent<sup>1</sup>; <sup>1</sup>Sandia National Labs, Albuquerque, New Mexico; <sup>2</sup>NIST, Gaithersburg, Maryland; <sup>3</sup>Northeastern University, Boston, Massachusetts; <sup>4</sup>Bogazici University, Istanbul, Turkey.

5:15 PM **E5.05**

**Observing Hydrophobic Water Pathways in Ion Channels** Ella Mihailescu<sup>1</sup>, Joseph Blasic<sup>2</sup> and David Worcester<sup>3</sup>; <sup>1</sup>Institute for Bioscience and Biotechnology Research, University of Maryland, Rockville, Maryland; <sup>2</sup>Biomolecular Measurement Division, National Institute for Standards and Technology, Gaithersburg, Maryland; <sup>3</sup>Physiology and Biophysics, University of California, Irvine, California.

SESSION EP4: Poster Session IV: Biology  
Wednesday Evening, June 4, 2014  
5:30 PM  
Summit II

**EP4.01**

**Bilayer Thickness Mismatch Controls Domain Size in Model Membranes** Frederick Heberle<sup>1</sup>, Robin Petrucciolo<sup>2</sup>, Jianjun Pan<sup>1</sup>, Paul Drazba<sup>3</sup>, Norbert Kucerka<sup>4</sup>, Robert Standaert<sup>1,3</sup>, Gerald Feigenson<sup>2</sup> and John Katsaras<sup>1,3</sup>; <sup>1</sup>ORNL, Oak Ridge, Tennessee; <sup>2</sup>Cornell University, Ithaca, New York; <sup>3</sup>The University of Tennessee, Knoxville, Tennessee; <sup>4</sup>Canadian Neutron Beam Centre, Chalk River, Ontario, Canada.

**EP4.02**

**Association of Model Neurotransmitters with Lipid Bilayer Membranes** Frank Heinrich<sup>1,2</sup>, Brian Josey<sup>1</sup>, Stefanie Rintoul<sup>3</sup>, Robert S. Cantor<sup>4</sup> and Mathias Loesche<sup>1,2,3</sup>; <sup>1</sup>Department of Physics, Carnegie Mellon, Pittsburgh, Pennsylvania; <sup>2</sup>NIST Center for Neutron Research (NCNR), Gaithersburg, Maryland; <sup>3</sup>Department of Biomedical Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania; <sup>4</sup>Department of Chemistry, Dartmouth College, Hanover, New Hampshire.

**EP4.03**

**Cracking the Structure of Cocaine** Andrew J. Johnston, Sylvia E. McLain and Sebastian Busch; Biochemistry, University of Oxford, Oxford, United Kingdom.

**EP4.04**

**Biophysical Study of the Dependence of Fusion of Dengue Virus with Host Membranes on Lipid Composition** Frank Heinrich<sup>2,4</sup>, Bulent Akgun<sup>5</sup>, David M. Rogers<sup>3</sup>, Juan M. Vanegas<sup>1</sup>, Bryan Carson<sup>1</sup>, Aihua Zheng<sup>6</sup>, Sushil Satija<sup>4</sup>, Margaret C. Kielian<sup>6</sup>, Susan L. Rempe<sup>1</sup> and Michael S. Kent<sup>1</sup>; <sup>1</sup>Sandia National Labs, Albuquerque, New Mexico; <sup>2</sup>Carnegie Mellon University, Pittsburgh, Pennsylvania; <sup>3</sup>University of South Florida, Tampa, Florida; <sup>4</sup>NIST, Gaithersburg, Maryland; <sup>5</sup>Bogazici Universities, Kimya Bolumu, Istanbul, Turkey; <sup>6</sup>Albert Einstein College of Medicine, New York, New York.

**EP4.05**

**Investigation of Water Dynamics in a Model Cellulosic System** Hugh O'Neill, Loukas Petridis, Junhong He, Barbara Evans, Eugene Mamontov, Liang Hong, Volker Urban, Brian Davison, Jeremy Smith and Paul Langan; ORNL, Oak Ridge, Tennessee.

**EP4.06**

**Simulation and Structure of Cel7A During Binding and Hydrolysis of Cellulose** Sai Venkatesh Pingali<sup>1</sup>, Junhong He<sup>1</sup>, Hugh M. O'Neill<sup>1</sup>, Volker S. Urban<sup>1</sup>, Loukas Petridis<sup>1</sup>, William T. Heller<sup>1</sup>, Marcus Foston<sup>2</sup>, Arthur J. Ragauskas<sup>2</sup>, Barbara R. Evans<sup>1</sup>, Jeremy C. Smith<sup>1</sup>, Paul Langan<sup>1</sup> and Brian H. Davison<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Institute of Paper Science and Technology, Georgia Institute of Technology, Atlanta,

Georgia.

**EP4.07**

**Photoactivation of a GPCR Rhodopsin Studied by Small Angle Neutron Scattering** Utsab Shrestha<sup>1</sup>, Kurt W. Van Delinder<sup>1</sup>, Suchithranga Perera<sup>2</sup>, Udeep Chawla<sup>2</sup>, Andrey V. Struts<sup>2</sup>, Shuo Qian<sup>3</sup>, William T. Heller<sup>3</sup>, Michael F. Brown<sup>2</sup> and Xiang-Qiang Chu<sup>1</sup>; <sup>1</sup>Department of Physics and Astronomy, Wayne State University, Detroit, Michigan; <sup>2</sup>Department of Chemistry and Biochemistry, University of Arizona, Tucson, Arizona; <sup>3</sup>Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

**EP4.08**

**Development of a Protein Expression and Purification Pipeline** Qiu Zhang, Venu Vandavasi, Kevin Weiss, Hugh O'Neill and Paul Langan; ORNL, Oak Ridge, Tennessee.



# F: Materials Chemistry and Materials for Energy

\* Invited paper

SESSION FP1: Poster Session I: Materials Chemistry and Materials for Energy  
Sunday Evening, June 1, 2014  
5:00 PM  
Summit II

## FP1.01

### The Ferromagnetic Domain Characteristics of FeRhPd Thin Films Probed by Polarized Neutron Scattering

Steven Bennett<sup>1</sup>, Haile Ambaye<sup>1</sup>, Hwachol Lee<sup>2</sup>, Patrick LeClair<sup>2</sup>, Gary Mankey<sup>2</sup> and Valeria Lauter<sup>1</sup>; <sup>1</sup>Quantum Condensed Matter Division, ORNL, Oak Ridge, Tennessee; <sup>2</sup>Department of Physics and Astronomy, University of Alabama, Tuscaloosa, Alabama.

## FP1.02

Unraveling Ordering Structures of LiNi<sub>0.5</sub>Mn<sub>1.5</sub>O<sub>4</sub> Cathode by Neutron Diffraction and Computer Simulation Yan Chen<sup>1</sup>, Yongqiang Cheng<sup>1</sup>, Mikhail Feyngenson<sup>1</sup>, Chengdu Liang<sup>2</sup> and Ke An<sup>1</sup>; <sup>1</sup>Chemical and Engineering Materials Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## FP1.03

Nano-Meso Scale Structure-Functional Transformation of Alkyl Substituted Polythiophenes During Aggregation Ilia Ivanov, Jiahua Zhu, Michael Stanford, Peter Bonnesen, Bobby Sumpter and Kunlun Hong; Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## FP1.04

Structural Characterization of n- and p-Type Skutterudite Thermoelectric Materials for Automotive Waste Heat Recovery Melanie Kirkham<sup>1</sup>, Hsin Wang<sup>2</sup>, Thomas R. Watkins<sup>2</sup>, E. A. Payzant<sup>1</sup>, J. R. Salvador<sup>3</sup>, G. P. Meisner<sup>3</sup>, A. J. Thompson<sup>4</sup> and J. W. Sharp<sup>4</sup>; <sup>1</sup>Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>General Motors Global R&D Center, Warren, Michigan; <sup>4</sup>Marlow Industries, Dallas, Texas.

## FP1.05

Multistep Topochemical Intercalation for the Formation of the Novel Layered Perovskites (A<sub>2</sub>ChH)LaNb<sub>2</sub>O<sub>7</sub> (Ch = Chalcogenides) John B Wiley and Dariush Montasserasadi; Chemistry, University of New Orleans, New Orleans, Louisiana.

## FP1.06

Impact of Physical Structure of Polymer on Miscibility of PCBM Siddharth Pradhan<sup>1</sup>, Mark Dadmun<sup>1</sup>, Huipeng Chen<sup>1</sup> and Nikos Kopidakis<sup>2</sup>; <sup>1</sup>University of Tennessee - Knoxville, Knoxville, Tennessee; <sup>2</sup>National Renewable Energy Laboratory, Denver, Colorado.

## FP1.07

Quantum Simulations of Inelastic Neutron Scattering Spectrum for H<sub>2</sub>/HD Molecule Inside the Nanocavities from Clathrate Hydrate to C<sub>60</sub> and Solid C<sub>60</sub>: Quantitative Comparison with Experiments Minzhong Xu, Anna Power, Shufeng Ye and Zlatko Bacic; Chemistry, New York University, New York, New York.

SESSION F1: Energy Conversion and Storage I  
Session Chair: Angus Wilkinson  
Monday Afternoon, June 2, 2014  
Tennessee Ballroom C

## 1:45 PM \*F1.01

Neutron Reflectometry Fitting Techniques for Under-Determined, Multi-Layered Structures: Lamellar Phase Segregation in Ultra-Thin Nafion Films Steven C. DeCaluwe<sup>1,2</sup>, Joseph A. Dura<sup>2</sup> and Paul A. Kienzie<sup>2</sup>; <sup>1</sup>Mechanical Engineering, Colorado School of Mines, Golden, Colorado; <sup>2</sup>Center for Neutron Research, NIST, Gaithersburg, Maryland.

## 2:15 PM F1.02

Neutron Reflection on a Cathode Electrode in a Functional Lithium-Ion Battery Brian Kitchen<sup>1</sup>, Joseph Dura<sup>2</sup> and Steven DeCaluwe<sup>3</sup>; <sup>1</sup>Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, Michigan; <sup>2</sup>NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland; <sup>3</sup>Mechanical Engineering, Colorado School of Mines, Golden, Colorado.

## 2:30 PM F1.03

Bulk and Interfacial Studies of Battery Electrode Materials Craig Bridges<sup>1</sup>, Xiaoguang Sun<sup>1</sup>, Zhonghe Bi<sup>1</sup>, Raymond Unocic<sup>2</sup>, Gabriel Veith<sup>2</sup>, Jinkui Zhao<sup>3</sup>, William Heller<sup>3</sup>, M. Parans Paranthaman<sup>1</sup> and Sheng Dai<sup>1</sup>; <sup>1</sup>Chemical Sciences Division, ORNL, Oak Ridge, Tennessee; <sup>2</sup>Materials Science and Technology Division, ORNL, Oak Ridge, Tennessee; <sup>3</sup>Spallation Neutron Source, ORNL, Oak Ridge, Tennessee.

## 2:45 PM F1.04

Probing the Liquid-Solid Interface of Lithium-Ion Batteries Gabriel M. Veith<sup>1</sup>, James F. Browning<sup>2</sup> and Jong Keum<sup>2</sup>; <sup>1</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## 3:00 PM F1.05

Pair Distribution Analysis of Garnet-Type Solid Electrolyte Li<sub>5</sub>La<sub>3</sub>Ta<sub>2</sub>O<sub>12</sub> Yuxing Wang<sup>1</sup>, Katharine Page<sup>2</sup> and Wei Lai<sup>1</sup>; <sup>1</sup>Chemical Engineering and Materials Science, Michigan State University, East Lansing, Michigan; <sup>2</sup>Lujan Neutron Scattering Center, Los Alamos National Laboratory, Los Alamos, New Mexico.

## 3:15 PM F1.06

Dependence of Li-Ion Conductivity and Activation Energies on the Crystal Structure and Ionic Radii in Li<sub>6</sub>MLa<sub>2</sub>Ta<sub>2</sub>O<sub>12</sub> Wolfgang G. Zeier<sup>1</sup>, Shiliang C. Zhou<sup>1</sup>, Beatriz C. Lopez-Bermudez<sup>1</sup>, Katharine Page<sup>2</sup> and Brent C. McIot<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Southern California, Los Angeles, California; <sup>2</sup>Lujan Neutron Scattering Center, Los Alamos National Laboratory, Los Alamos, New Mexico.

## 3:30 PM BREAK

SESSION F2: Inelastic and Quasielastic Studies of Materials  
Session Chair: Stewart Parker  
Monday Afternoon, June 2, 2014  
Tennessee Ballroom C

## 4:00 PM \*F2.01

Hydration Layers on Metal-Oxide Nanoparticles: Insights from Inelastic Neutron Scattering Nancy Ross, Geosciences, Virginia Tech, Blacksburg, Virginia.

## 4:30 PM F2.02

Ion Migration Processes in Lanthanum Barium Gallate Studied by Neutron Scattering Niina Jalarvo<sup>1,2</sup>, Olivier Gourdon<sup>3</sup>, Laura Stingaciu<sup>1</sup>, Zhonghe Bi<sup>4</sup>, Delphine Gout<sup>3</sup>, Michael Ohl<sup>1</sup> and M. Parans Paranthaman<sup>4</sup>; <sup>1</sup>Juelich Centre for Neutron Science, Outstation at Spallation Neutron Source, Research Centre Juelich, Oak Ridge, Tennessee; <sup>2</sup>Chemical and Engineering Materials Division, Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Lujan Center (LANSCE-LC), Los Alamos National Laboratory, Los Alamos, New Mexico; <sup>4</sup>Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## 4:45 PM F2.03

The Selection Rules in Inelastic Neutron Scattering for Molecular Translational and Rotational Spectroscopy Minzhong Xu, Shufeng Ye and Zlatko Bacic; Chemistry, New York University, New York, New York.

## 5:00 PM F2.04

Dynamics of Propane Absorbed in Nanoporous Silica Aerogel: Quasielastic Neutron Scattering Study Siddharth S. Gautam<sup>1</sup>, Tingting Liu<sup>1</sup>, Gernot Rother<sup>2</sup>, Niina Jalarvo<sup>3,4</sup>, Eugene Mamontov<sup>4</sup>, Susan Welch<sup>1</sup>, Michael Droegge<sup>5</sup> and David Cole<sup>1</sup>; <sup>1</sup>School of Earth Sciences, The Ohio State University, Columbus, Ohio; <sup>2</sup>Geochemistry and Interfacial Science Group, Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Juelich Centre for Neutron Science (JCNS-1), Outstation at Spallation Neutron Source (SNS), Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Chemical and Engineering Materials Division, Neutron Sciences

Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee;  
<sup>5</sup>Ocellus Inc, Livermore, California.

#### 5:15 PM **F2.05**

**Tunneling and Vibrational Dynamics of Ultra-Confined Water** Alexander I. Kolesnikov<sup>1</sup>, Lawrence M. Anovitz<sup>2</sup>, Eugene Mamontov<sup>1</sup>, Andrey Podlesnyak<sup>3</sup> and Georg Ehlers<sup>3</sup>; <sup>1</sup>Chemical and Engineering Materials Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

SESSION FP2: Poster Session II: Materials Chemistry  
and Materials for Energy  
Monday Evening, June 2, 2014  
5:30 PM  
Summit II

#### **FP2.01**

**Neutron Scattering Study of Thin Films of Molecular Hydrogen on MgO(100) Surfaces** Sourav Adak<sup>1</sup>, Tilo Seydel<sup>2</sup>, Georg Ehlers<sup>3</sup> and John Z. Larese<sup>1</sup>; <sup>1</sup>Chemistry, University of Tennessee, Knoxville, Tennessee; <sup>2</sup>Institut Laue Langevin, Grenoble, France; <sup>3</sup>Spallation Neutron Source, ORNL, Oak Ridge, Tennessee.

#### **FP2.02**

**More Examples of Atomic Hirshfeld Surface Analysis in Non-Molecular Crystals** Bryan C. Chakoumakos<sup>1</sup>, Huibo Cao<sup>1</sup> and Parthapratim Munshi<sup>2</sup>; <sup>1</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Department of Chemistry & Center for Informatics, Shiv Nadar University, Tehsil Dadri, Uttar Pradesh, India.

#### **FP2.03**

**Novel Low-Scattering Solvents for *In – Operando* Neutron Diffraction in Electrochemical Cells** Tyler M. Fears<sup>1</sup>, Nicholas Leventis<sup>1</sup>, Chariklia Sotiriou-Leventis<sup>1</sup>, Jeffrey G. Winiarz<sup>1</sup>, Helmut Kaiser<sup>2,3</sup> and Haskell Taub<sup>3,2</sup>; <sup>1</sup>Department of Chemistry, Missouri University of Science and Technology, Rolla, Missouri; <sup>2</sup>University of Missouri Research Reactor, University of Missouri, Columbia, Missouri; <sup>3</sup>Department of Physics and Astronomy, University of Missouri, Columbia, Missouri.

#### **FP2.04**

**Comparison of X-Ray Diffraction (XRD) and Neutron Diffraction Characterization on Fe<sub>16</sub>N<sub>2</sub> Bulk Magnet Material** Yanfeng Jiang<sup>1</sup>, Xiaowei Zhang<sup>1</sup>, Valeria Lauter<sup>2</sup> and Jian-Ping Wang<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, Minnesota; <sup>2</sup>Oak Ridge National Laboratory, Knoxville, Tennessee.

#### **FP2.05**

**Structure and Magnetic Properties of a Ferromagnetic Insulating Framework Material, Ba<sub>x</sub>(M<sup>III</sup><sub>y</sub>Mn<sub>1-y</sub>)O<sub>2</sub>** Amber Larson and Efrain Rodriguez; Department of Chemistry & Biochemistry, University of Maryland, College Park, Maryland.

#### **FP2.06**

**Competing Superexchange Interactions in Double Perovskite Osmates** Ryan C. Morrow and Patrick M. Woodward; Chemistry, Ohio State University, Columbus, Ohio.

#### **FP2.07**

**Graphene-Based ‘Hybrid’ Nanomaterials with Manganese Oxides for Alternative Clean Energy: Synthesis and Structural Properties** M. M. Van Mevren<sup>1</sup>, J. Jasinski<sup>2</sup> and Sanju Gupta<sup>1</sup>; <sup>1</sup>Physics and Astronomy, Western Kentucky University, Bowling Green, Kentucky; <sup>2</sup>Conn Center for Renewable Energy, University of Louisville, Louisville, Kentucky.

#### **FP2.08**

**The Lattice Strain Response to Characterize the New Mechanisms on Superelastic Behavior of Pre-Martensite for NiFeGaCo Shape Memory Alloy** Hui Yang, Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee.

SESSION F3: Functional Oxide Materials  
Session Chair: Anna Llobet Megias  
Tuesday Morning, June 3, 2014  
Tennessee Ballroom C

#### 10:15 AM **\*F3.01**

**Representational Analysis of Extended Disorder in Functional Oxides** James R. Neilson, Chemistry, Colorado State University, Fort

Collins, Colorado.

#### 10:45 AM **\*F3.02**

**Mixed-Valence Microporous Oxides for Magnetic Properties and Energy Conversion** Amber M. Larson, Pouya Moetakef and Efrain E. Rodriguez; Chemistry and Biochemistry, University of Maryland, College Park, Maryland.

#### 11:15 AM **F3.03**

**Neutron Diffraction and RMC Modeling of New Amorphous Molybdate System** Margit Fabian<sup>1,2</sup>, Claudia Pantalei<sup>3</sup>, Kiril Krezhov<sup>4</sup> and Erzsebet Svab<sup>2</sup>; <sup>1</sup>Centre for Energy Research, Budapest, Hungary; <sup>2</sup>Wigner Research Centre for Physics, Budapest, Hungary; <sup>3</sup>Laboratoire Leon Brillouin, Saclay, France; <sup>4</sup>Institute for Nuclear Research and Nuclear Energy, Sofia, Bulgaria.

#### 11:30 AM **F3.04**

**Averaged and Local Crystal Structure of GaN/ZnO Solid Solution Nanoparticles** Mikhail Feyngenson<sup>1</sup> and Weiqiang Han<sup>2</sup>; <sup>1</sup>Chemical and Engineering Materials Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Division of New Energy, Ningbo Institute of Materials Technology and Engineering, Ningbo, China.

#### 11:45 AM **F3.05**

**Ferroelectric, Piezoelectric and Structural Studies of Novel Bi-Based Perovskites** Michelle Dolgos, Chemistry, Oregon State University, Corvallis, Oregon.

#### 12:00 PM **F3.06**

**Phonon Localization as a Driver for Polar Nanoregions in Relaxor Ferroelectrics** Michael E. Manley<sup>1</sup>, Jeffrey W. Lynn<sup>2</sup>, Douglas Abernathy<sup>1</sup>, Eliot D. Specht<sup>1</sup>, Olivier Delaire<sup>1</sup>, Alan Bishop<sup>3</sup>, Raffi Sahul<sup>4</sup> and John D. Budai<sup>1</sup>; <sup>1</sup>Scattering and Thermophysics Group, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>NIST Center for Neutron Scattering, National Institute of Science and Technology, Gaithersburg, Maryland; <sup>3</sup>Los Alamos National Laboratory, Los Alamos, New Mexico; <sup>4</sup>TRS Technologies, State College, Pennsylvania.

SESSION FP3: Poster Session III: Materials Chemistry  
and Materials for Energy  
Tuesday Afternoon, June 3, 2014  
3:30 PM  
Summit II

#### **FP3.01**

**Detection of Trapped Nanobubbles on Nanostructured Surfaces having Different Wettability: A SANS Investigation** Jitendra Bahadur<sup>1</sup>, Yuri B. Melnichenko<sup>1</sup>, Nikolay V. Lavrik<sup>2</sup>, Emilian Popov<sup>3</sup>, Lilin He<sup>1</sup>, Ivan I. Kravchenko<sup>2</sup>, Gregory S. Smith<sup>1</sup>, Vitaliy Pipich<sup>4</sup> and Noemi Szekeley<sup>4</sup>; <sup>1</sup>Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Reactor and Nuclear Systems Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Forschungszentrum Juelich GmbH, Garching, Germany.

#### **FP3.02**

**Preparation of Functional Composite by Decoration of Metal Nanoparticles on Graphene** Lilei Chen, Huaqing Xie, Min Cheng and Dejun Yang; Shanghai Second Polytechnic University, Shanghai, China.

#### **FP3.03**

**Use of Neutron Diffraction to Characterize Cold Rolled Zircaloy – 4 Powder** Jacques Huot<sup>1</sup>, Ivaldette d. Dupim<sup>2</sup>, Sydney F. Santos<sup>2</sup> and Roxana Flacau<sup>3</sup>; <sup>1</sup>UQTR, Trois-Rivieres, Quebec, Canada; <sup>2</sup>UFABC, Santo Andre, Sao Paulo, Brazil; <sup>3</sup>Chalk River Laboratories, National Research Council Canada, Chalk River, Ontario, Canada.

#### **FP3.04**

**Effects of Pressure on Microstructure Network in Thermoelectric (Bi,Sb)<sub>2</sub>Te<sub>3</sub>** Hye J. Kang<sup>1</sup>, Menghan Zhou<sup>1</sup>, Wenjie Xie<sup>2</sup> and Boualem Hammouda<sup>3</sup>; <sup>1</sup>Physics & Astronomy, Clemson University, Clemson, South Carolina; <sup>2</sup>Wuhan University of Technology, Wuchang, Wuhan, China; <sup>3</sup>National Institute of Standards & Technology, Gaithersburg, Maryland.

#### **FP3.05**

**A Structural Characterization of Lignin-Based Composite Anodes for Lithium-Ion Batteries** Nicholas McNutt<sup>1</sup>, Marshall McDonnell<sup>1</sup>, Orlando Rios<sup>2</sup>, Mikhail Feyngenson<sup>3</sup> and David Keffer<sup>4</sup>; <sup>1</sup>Chemical & Biomolecular Engineering, University of Tennessee,

Knoxville, Tennessee; <sup>2</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Chemical and Engineering Materials Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>4</sup>Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee.

#### FP3.06

##### **Correlating Neutron Scattering and Atomic-Resolution Microscopy to Characterize Radiation-Tolerant Alloys**

Chad Parish<sup>1</sup>, Xun-Li Wang<sup>2,1</sup>, Zhongwu Zhang<sup>3,1</sup> and Michael Miller<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>City University of Hong Kong, Hong Kong, Hong Kong; <sup>3</sup>Harbin Engineering University, Harbin, China.

#### FP3.07

##### **Molecular Simulations of Gold Nanotips in Dithiol Solvent**

Huachuan Wang, George Washington University, Washington, District of Columbia.

#### FP3.08

**Dynamics of Thermo- and Solvato- Chromic Behaviour of Brush Block Polymers of Polythiophenes.** Jiahua Zhu, Suk-kyun Ahn, Iliia Ivanov and Kunlun Hong; Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

SESSION F4: Energy Conversion and Storage II

Session Chair: Efrain Rodriguez

Wednesday Afternoon, June 4, 2014

Tennessee Ballroom C

#### 1:45 PM \*F4.01

##### **Inelastic Neutron Scattering Measurements and Computer Simulations of Phonons in Thermoelectric Materials**

Olivier Delaire, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### 2:15 PM F4.02

##### **Phonon Self-Energy and Origin of Anomalous Neutron Scattering Spectra in SnTe and PbTe Thermoelectrics**

Chen Li<sup>1</sup>, Olle Hellman<sup>2</sup>, Jie Ma<sup>3</sup>, Andrew F. May<sup>1</sup>, Huibo Cao<sup>3</sup>, Xin Chen<sup>1</sup>, Andrew D. Christianson<sup>3</sup>, Georg Ehlers<sup>3</sup>, David J. Singh<sup>1</sup>, Brian C. Sales<sup>1</sup> and Olivier Delaire<sup>1</sup>; <sup>1</sup>Material Science and Technology Division, Oak Ridge National Laboratory, Knoxville, Tennessee; <sup>2</sup>Department of Physics, Chemistry and Biology, Linköping University, Linköping, Sweden; <sup>3</sup>Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### 2:30 PM \*F4.03

**Insights Into Solid Oxide Fuel Cell Materials by In-Situ Neutron Diffraction** Steven McIntosh, Chemical Engineering, Lehigh University, Bethlehem, Pennsylvania.

#### 3:00 PM F4.04

**Methane Hydrate Formation in the Presence of Clay Nanoparticles** Diana Taylor and Neal Skipper; London Centre for Nanotechnology, UCL, London, United Kingdom.

#### 3:15 PM F4.05

**Structure of Nafion Nanocomposite Membranes for Vanadium Redox Flow Batteries** Eric M. Davis and Kirt A. Page; Materials Science and Engineering, National Institute of Standards & Technology, Gaithersburg, Maryland.

#### 3:30 PM BREAK

SESSION F5: Materials Chemistry I

Session Chair: Stephen Decaluwe

Wednesday Afternoon, June 4, 2014

Tennessee Ballroom C

#### 4:00 PM F5.01

##### **Assisted Phase-Separation in Polymer-Based Solar Cells by Silica Particles** Hao Shen<sup>1</sup>, Michael E. Mackay<sup>1,2</sup> and Yun Liu<sup>1,3</sup>;

<sup>1</sup>Chemical and Biomolecular Engineering, University of Delaware, Newark, Delaware; <sup>2</sup>Materials Science and Engineering, University of Delaware, Newark, Delaware; <sup>3</sup>NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland.

#### 4:15 PM F5.02

**The Isotopic Effects of Deuteration on the Optoelectronic Properties of Conducting Polymers** Kai Xiao<sup>1</sup>, Ming Shao<sup>1</sup>, Jong Keum<sup>1,2</sup>, Kunlun Hong<sup>1</sup>, Jim Browning<sup>2</sup>, Jihua Chen<sup>1</sup>, Jacek Jakowski<sup>3</sup> and David Geoghegan<sup>1</sup>; <sup>1</sup>Center for Nanophase Materials

Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Chemical and Engineering Materials Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>National Institute of Computational Sciences, University of Tennessee, Oak Ridge, Tennessee.

#### 4:30 PM F5.03

##### **Effect of P3HT Molecular Weight on the Morphology, Miscibility and Photovoltaic Properties of P3HT:PCBM Mixtures in Organic Photovoltaics** Huipeng Chen<sup>1</sup>, Siddharth

Pradhan<sup>1</sup>, Nikos Kopidakis<sup>2</sup>, Andrew Ferguson<sup>2</sup> and Mark Dadmun<sup>1,3</sup>; <sup>1</sup>Chemistry, University of Tennessee, Knoxville, Tennessee; <sup>2</sup>National Renewable Energy Laboratory, Golden, Colorado; <sup>3</sup>Chemical Sciences Division, Oak Ridge, Tennessee.

#### 4:45 PM F5.04

**Characterizing Highly-Loaded Carbon Nanotube Polymer Nanocomposites with SANS and USANS** Mehran Tchrani<sup>1</sup> and Mark Dadmun<sup>2,3</sup>; <sup>1</sup>Mechanical Eng., Univ. of New Mexico, Albuquerque, New Mexico; <sup>2</sup>Department of Chemistry, University of Tennessee, Knoxville, Tennessee; <sup>3</sup>Chemical Sciences Division, Oak Ridge National Lab, Oak Ridge, Tennessee.

#### 5:00 PM F5.05

##### **Morphology and Hydrogen Adsorption Capacity of**

**Nanoporous Carbons** Lilin He<sup>1</sup>, Cristian I. Contescu<sup>2</sup>, Yuri B. Melnichenko<sup>1</sup>, Junjie Guo<sup>2</sup>, Nidia C. Gallego<sup>2</sup> and Jitendra Bahadur<sup>1</sup>; <sup>1</sup>Biology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### 5:15 PM F5.06

##### **Quantum Sieving of Hydrogen Isotopes Confined in Carbon**

**Nanopores** Cristian I. Contescu<sup>1</sup>, James R. Morris<sup>1</sup>, Eugene Mamontov<sup>2</sup>, Raina J. Olsen<sup>1</sup> and Nidia C. Gallego<sup>1</sup>; <sup>1</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Chemical and Engineering Materials Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

SESSION FP4: Poster Session IV: Materials Chemistry and Materials for Energy

Wednesday Evening, June 4, 2014

5:30 PM

Summit II

#### FP4.01

##### **Vibrational Dynamics of Ammonia, Doped in a Barium Iron Selenide Superconductor** Stuart I. Campbell<sup>1</sup>, Alexander I.

Kolesnikov<sup>2</sup>, Jonathan E. Mitchell<sup>3</sup>, Athena S. Sefat<sup>3</sup> and Garrett E. Granroth<sup>1</sup>; <sup>1</sup>Neutron Data Analysis and Visualization, ORNL, Oak Ridge, Tennessee; <sup>2</sup>Chemical and Engineering Materials Division, ORNL, Oak Ridge, Tennessee; <sup>3</sup>Materials Science and Technology Division, ORNL, Oak Ridge, Tennessee.

#### FP4.02

##### **Interpreting INS Spectra Using Computer Simulation: The**

**Integrated Approach at VISION** Yongqiang Cheng, Anibal (Timmy) Ramirez-Cuesta, Christoph Wildgruber and Lacy Jones; Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### FP4.03

##### **From Graphite to Graphene: Direct Liquid-Phase Exfoliation**

**Producing Mono-, Bi-, and Oligo- Layered Graphene** Aline Irihamye, C. Price, E. Heintzman and Sanju Gupta; Physics and Astronomy, Western Kentucky University, Bowling Green, Kentucky.

#### FP4.04

##### **INS Studies of Small Molecule Interaction with Transition**

**Aluminas** John Z. Larese<sup>1</sup>, Sourav Adak<sup>1</sup>, Chuck Sumner<sup>2</sup> and Luke L. Daemen<sup>3</sup>; <sup>1</sup>Chemistry, University of Tennessee, Knoxville, Tennessee; <sup>2</sup>Eastman Chemical, Kingsport, Tennessee; <sup>3</sup>Los Alamos National Laboratory, Los Alamos, New Mexico.

#### FP4.05

##### **Influence of Light Absorption on the Chain Conformation of Conjugated Polymers** Brian Morgan and Mark Dadmun;

Chemistry, University of Tennessee Knoxville, Knoxville, Tennessee.

#### FP4.06

##### **Identifying Morphology in High Performance Facilitated**

**Transport, Hydroxide-Exchange Membranes** Laj Xiong<sup>1</sup>, Hao Shen<sup>1</sup>, Yushan Yan<sup>1</sup> and Yun Liu<sup>1,2</sup>; <sup>1</sup>Chemical and Biomolecular Engineering, University of Delaware, Newark, Delaware; <sup>2</sup>NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland.

#### **FP4.07**

**Theoretical Investigation on Thermal Properties of Single-Walled Carbon Nanotubes Composite** Jifen Wang,  
Shanghai Second Polytechnic University, Shanghai, China.

#### **SESSION F6: Materials Chemistry II**

Session Chair: Nancy Ross

Thursday Morning, June 5, 2014

Tennessee Ballroom C

#### **9:45 AM \*F6.01**

**Total Scattering Descriptions Reveal Local Distortions in Oxide "Solid Solutions"** Daniel Shoemaker, Materials Science and Engineering, University of Illinois, Urbana, Illinois.

#### **10:15 AM F6.02**

**Structure and Dynamics of the Superprotonic Conductor CsHSO<sub>4</sub>** Stewart F. Parker and Samantha K. Callear; ISIS Facility, STFC Rutherford Appleton Laboratory, Didcot, Oxon, United Kingdom.

#### **10:30 AM F6.03**

**Diffusive and Rotational Dynamics of *n*-H<sub>2</sub> Confined in MCM-41** Timothy Prisk, Matthew Bryan and Paul Sokol; Department of Physics, Indiana University, Bloomington, Indiana.

#### **10:45 AM F6.04**

**Structure-Property Relations of Cation-Exchanged CHA, and KFI-Type Zeolites for CO<sub>2</sub> Adsorption** Trong Pham<sup>1</sup>, Craig Brown<sup>1,2</sup>, Matthew Hudson<sup>2</sup> and Raul Lobo<sup>1</sup>; <sup>1</sup>Chemical and Biomolecular Engineering, Univ of Delaware, NEWARK, Delaware; <sup>2</sup>Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland.

#### **11:00 AM F6.05**

**Nematic Order and the Recovery of Magnetic Degeneracy in Iron-Based Superconductors** Omar Chmaissem<sup>1,2</sup>, Sevda Avci<sup>2</sup>, Stephan Rosenkranz<sup>2</sup>, Jared Allred<sup>2</sup>, Raymond Osborn<sup>2</sup>, Ilya Eremin<sup>3</sup>, Andrey V. Chubukov<sup>4</sup>, Duck Young Chung<sup>2</sup>, Mercouri Kanatzidis<sup>5</sup>, Helmut Claus<sup>2</sup>, Dmitry D. Khalyavin<sup>6</sup>, Pascal Manuel<sup>6</sup> and Aziz Daoud-Aladine<sup>6</sup>; <sup>1</sup>Department of Physics, Northern Illinois University, DeKalb, Illinois; <sup>2</sup>Materials Science Division, Argonne National Laboratory, Argonne, Illinois; <sup>3</sup>Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Germany; <sup>4</sup>Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin; <sup>5</sup>Department of Chemistry, Northwestern University, Evanston, Illinois; <sup>6</sup>ISIS Pulsed Neutron and Muon Facility, Rutherford Appleton Laboratory, Didcot, United Kingdom.

#### **11:15 AM F6.06**

**On the Origin of First Sharp Diffraction Peak in Arsenic Selenide Glasses** Justin Oelgoetz<sup>1</sup>, Roman Golovchak<sup>1</sup>, Andriy Kovalsky<sup>1</sup>, Mikhail Feygenson<sup>2</sup> and Joerg Neuefeind<sup>2</sup>; <sup>1</sup>Physics and Astronomy, Austin Peay State University, Clarksville, Tennessee; <sup>2</sup>SNS, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

# G: Engineering and Industrial Applications

\* Invited paper

SESSION GP1: Poster Session I: Engineering and Industrial Applications  
Monday Evening, June 2, 2014  
5:30 PM  
Summit II

## GP1.01

### iMars (iMaging Analysis and Reduction Software)

Jean Bilheux, Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## GP1.02

**Measurement and Simulation of Residual Stress in Additive Manufacturing** Le Tao<sup>1</sup>, John Hasler<sup>1</sup>, Philip Nash<sup>1</sup> and Bjørn Clausen<sup>2</sup>; <sup>1</sup>Thermal Processing Technology Center, Illinois Institute of Technology, Chicago, Illinois; <sup>2</sup>Lujan Center, LANCE, Los Alamos National Laboratory, Los Alamos, New Mexico.

## GP1.03

### Accomplishments and Future Needs for Engineering Applications Using Energy Selective Neutron Imaging

Robin Woracek<sup>1,2</sup>, Dayakar Penumadu<sup>1</sup>, Nikolay Kardukov<sup>2</sup>, Ingo Manke<sup>2</sup>, Mirko Boin<sup>2</sup>, Andre Hilger<sup>2</sup> and Anton Tremsin<sup>3</sup>; <sup>1</sup>University of Tennessee, Knoxville, Tennessee; <sup>2</sup>Helmholtz Zentrum Berlin, Berlin, Germany; <sup>3</sup>University of California at Berkeley, Berkeley, California.

## GP1.04

### Residual Stresses in Friction Stir Welded ODS Alloys

Edward A. Payzant<sup>1</sup>, Lindsay M. Kolbus<sup>1</sup>, Luke N. Brewer<sup>2</sup> and Martin S. Bennett<sup>2</sup>; <sup>1</sup>ORNL, Oak Ridge, Tennessee; <sup>2</sup>Naval Postgraduate School, Monterey, California.

## GP1.05

**Neutron Determination of Hydrogen Concentration and Distribution: Correlation to Mechanical Properties of Hydrided Zr Alloy Cladding** Yong Yan, Shuo Qian, Ken Littrell, Hassina Bilheux, Jean-Christophe Bilheux, Holly Ray and Tyler Smith; Oak Ridge National Laboratory, Oak Ridge, Tennessee.

SESSION G1: Processing and Mechanical Properties  
Session Chair: Zhenzhen Yu  
Tuesday Morning, June 3, 2014  
Tennessee Ballroom A

## 10:30 AM \*G1.01

**Neutrons in the Oil Patch** Lynann Clapham<sup>1</sup>, Ronald Rogge<sup>2</sup> and Thomas Gnaeupel-Herold<sup>3</sup>; <sup>1</sup>Engineering Physics, Queen's University, Kingston, Ontario, Canada; <sup>2</sup>Canadian Neutron Beam Laboratory, Chalk River, Ontario, Ontario, Canada; <sup>3</sup>National Institute of Standards and Technology, Gaithersburg, Maryland.

## 11:00 AM \*G1.02

**In-Situ Neutron Diffraction for Advancing Constitutive Models of Shape Memory Alloys** Aaron Stebner, Mechanical Engineering, Colorado School of Mines, Golden, Colorado.

## 11:30 AM G1.03

**Load Transfer and Stress Relaxation in NiAl-Strengthened Ferritic Alloys** Zhiqian Sun<sup>1</sup>, Gian Song<sup>1</sup>, Thomas A. Sisneros<sup>2</sup>, Bjørn Clausen<sup>2</sup>, Donald W. Brown<sup>2</sup> and Peter K. Liaw<sup>1</sup>; <sup>1</sup>University of Tennessee, Knoxville, Tennessee; <sup>2</sup>Lujan Neutron Scattering Center, Los Alamos National Laboratory, Los Alamos, New Mexico.

## 11:45 AM G1.04

**Microstructural Evolution of Monolithic Fuel Foils During Processing** Bjørn Clausen<sup>1</sup>, Donald W. Brown<sup>2</sup>, Maria Okuniewski<sup>3</sup>, Levente Balogh<sup>4</sup> and Thomas A. Sisneros<sup>2</sup>; <sup>1</sup>Lujan Center, Los Alamos National Laboratory, Los Alamos, New Mexico; <sup>2</sup>MST-8, Los Alamos National Laboratory, Los Alamos, New Mexico; <sup>3</sup>Fundamental Fuel Properties, Idaho National Laboratory, Idaho Falls, Idaho; <sup>4</sup>Department of Mechanical and Materials Engineering, Queen's University, Kingston, Ontario, Canada.

## 12:00 PM G1.05

**Neutron Diffraction Stress Measurements on Suspension Bridge Wire Bundles – Effect on Wire Twist** Adrian Brugger<sup>1</sup>, Seung-Yub Lee<sup>2,3</sup>, Hande Ozturk<sup>2,3</sup>, Ajinkya J. Rajc<sup>1</sup> and Ismail C. Noyan<sup>2,3</sup>; <sup>1</sup>Civil Engineering & Engineering Mechanics, Columbia University, New York, New York; <sup>2</sup>Materials Science and Engineering, Columbia University, New York, New York; <sup>3</sup>Applied Physics and Applied Mathematics, Columbia University, New York, New York.

SESSION GP2: Poster Session II: Engineering and Industrial Applications  
Tuesday Afternoon, June 3, 2014  
3:30 PM  
Summit II

## GP2.01

### Effect of Selective Placement of CuO Nanostructures in an Oscillating Heat Pipe Studied with Neutron Imaging

Robert A. Winholtz<sup>1</sup>, Feng Zhang<sup>1</sup>, Michael Wilson<sup>1</sup>, Wolfgang Black<sup>1</sup>, Hongbin Ma<sup>1</sup>, Daniel Hussey<sup>2</sup> and David Jacobson<sup>2</sup>; <sup>1</sup>Mechanical and Aerospace Engineering, University of Missouri, Columbia, Missouri; <sup>2</sup>Physics Laboratory, National Institute of Standards and Technology, Gaithersburg, Maryland.

## GP2.02

**Spallation Neutron Source, Sample Environment High Temperature Program** Rebecca A. Mills and Douglas P. Armitage; NSCD Sample Environment, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## GP2.03

**Zirconium Hydride Phase Transformation in Zircaloy-4: Correlation to Ductility Changes as a Function of Temperature of Hydrided Zr Alloy Cladding** Ken Littrell, Yong Yan, Shuo Qian, Jordan Favret, Katie Andrews, Holly Ray and Tyler Smith; ORNL, Oak Ridge, Tennessee.

## GP2.04

### Studying Hydrogen Effects on the Deformation Behavior of Pipeline Steels by Neutron-Diffraction Measurements

Bilin Chen<sup>1</sup>, Ke An<sup>2</sup> and Peter K. Liaw<sup>1</sup>; <sup>1</sup>University of Tennessee, Knoxville, Tennessee; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## GP2.05

**Elastic Anisotropy of Nanostructured Ferritic Alloys at Elevated Temperatures** Alexandru D. Stoica<sup>1</sup>, Grigoreta M. Stoica<sup>1</sup>, Dong Ma<sup>1</sup> and Michael K. Miller<sup>2</sup>; <sup>1</sup>Chemical and Engineering Materials Division, ORNL, Oak Ridge, Tennessee; <sup>2</sup>Materials Science and Technology Division, ORNL, Oak Ridge, Tennessee.

SESSION G2: Dislocations, Diffusion and Flow  
Session Chair: Ken Littrell  
Wednesday Afternoon, June 4, 2014  
Tennessee Ballroom A

## 1:45 PM \*G2.01

**In-Situ Studies of Dislocation Structure Evolution During Annealing of Neutron Irradiated Zr-2.5Nb Alloy** Levente Balogh<sup>1</sup>, Donald W. Brown<sup>2</sup>, Bjørn Clausen<sup>3</sup>, Fei Long<sup>1</sup>, Paula Mosbrucker<sup>4</sup>, Thomas A. Sisneros<sup>2</sup> and Mark R. Daymond<sup>1</sup>; <sup>1</sup>Department of Mechanical and Materials Engineering, Queen's University, Kingston, Ontario, Canada; <sup>2</sup>Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, New Mexico; <sup>3</sup>Los Alamos Neutron Science Center, Los Alamos National Laboratory, Los Alamos, New Mexico; <sup>4</sup>Kinectrics Inc., Toronto, Ontario, Canada.

## 2:15 PM G2.02

**Fabrication of New Low Viscosity-Temperature Feedstock Using Nano-Sized Powder Stainless Steel 316L and An Environment-Friendly Binder in Micro Powder Injection Molding** Javad Rajabi, Norhamidi Muhamad, Abu B. Sulong and Abdolali Fayyaz; Mechanical and Materials Engineering, The National University of Malaysia, Bangi, Malaysia.

## 2:30 PM G2.03

**Quantification of the Temperature Dependence of Hydrogen Dislocation Pipe Diffusion in Deformed Pd Using QENS** Brent Heuser<sup>1</sup>, Dallas Trinkle<sup>2</sup>, Joseph Serio<sup>1</sup>, Emily Schiavone<sup>2</sup>, Niina Jalarvo<sup>3</sup> and Eugene Mamontov<sup>3</sup>; <sup>1</sup>Nuclear Engineering, University of Illinois, Urbana, Illinois; <sup>2</sup>Materials Science and

Engineering, University of Illinois, Urbana, Illinois; <sup>3</sup>SNS, ORNL, Oak Ridge, Tennessee.

#### **2:45 PM G2.04**

**Using Neutron Radiography to Accurately Quantify the Through-Plane Water Content of a Proton-Exchange Membrane** David L. Jacobson<sup>1</sup>, Devin O'Kelly<sup>4</sup>, Daniel S. Hussey<sup>1</sup>, Dusan Spornjak<sup>2</sup>, Adam Z. Weber<sup>3</sup>, Rangachary Mukundan<sup>2</sup>, Joseph Fairweather<sup>2</sup>, Jacob S. Spendlow<sup>2</sup> and Rodney L. Borup<sup>2</sup>; <sup>1</sup>Physical Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, Maryland; <sup>2</sup>Los Alamos National Laboratory, Los Alamos, New Mexico; <sup>3</sup>Environmental Energy Technologies Division, Lawrence Berkeley National Laboratory, Berkeley, California; <sup>4</sup>University of Texas at Austin, Austin, Texas.

#### **3:00 PM G2.05**

**Investigation of Deformation Dynamics in a Rolled Magnesium Alloy by Real-Time In-Situ Neutron Diffraction** Wei Wu<sup>1</sup>, Hua Qiao<sup>2</sup>, Peidong Wu<sup>2</sup>, Peter K. Liaw<sup>3</sup> and Ke An<sup>1</sup>; <sup>1</sup>Chemical and Engineering Materials, Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>2</sup>Department of Mechanical Engineering, McMaster University, Hamilton, Ontario, Canada; <sup>3</sup>Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee.

#### **3:15 PM G2.06**

**Modelling Neutron Attenuation Through Cement-Based Mortar** Catherine Lucero<sup>1</sup>, Dale P. Bentz<sup>2</sup>, Daniel S. Hussey<sup>2</sup>, David L. Jacobson<sup>2</sup> and W. J. Weiss<sup>1</sup>; <sup>1</sup>Civil Engineering, Purdue University, West Lafayette, Indiana; <sup>2</sup>Physical Measurements Laboratory, National Institute of Standards and Technology, Gaithersburg, Maryland.

SESSION GP3: Poster Session III: Engineering and Industrial Applications  
Wednesday Evening, June 4, 2014  
5:30 PM  
Summit II

#### **GP3.01**

**Pressure Variable Wide Angle Polarized 3He Analyzer System for the SNS Hybrid Spectrometer** Daniel R. Brown<sup>1</sup>, Xin Tong<sup>1</sup>, Chenyang Jiang<sup>1</sup>, Barry Winn<sup>1</sup>, Melissa Graves-Brook<sup>1</sup>, Lee Robertson<sup>1</sup> and Mark Haggen<sup>2</sup>; <sup>1</sup>ORNL-ORAU, Oak Ridge, Tennessee; <sup>2</sup>ESS, Lund, Sweden.

#### **GP3.02**

**Using Neutron Residual Strain Measurements and A Force Balance Method on Additively Manufactured Inconel 718** Lindsay M. Kolbus<sup>1</sup>, Edward A. Payzant<sup>1</sup>, Thomas R. Watkins<sup>2</sup> and Sudarsanam S. Babu<sup>2,3</sup>; <sup>1</sup>Chemical and Engineering Materials, Oak Ridge National Lab, Oak Ridge, Tennessee; <sup>2</sup>Materials Science and Technology, Oak Ridge National Lab, Oak Ridge, Tennessee; <sup>3</sup>Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee.

#### **GP3.03**

**Measuring the Magnetic State of an Artificial Skrymion Lattice with Specular and Near-Specular Scattering** Brian B. Maranville<sup>1</sup>, Dustin Gilbert<sup>2</sup>, Julie Borchers<sup>1</sup>, Brian Kirby<sup>1</sup> and Kai Liu<sup>2</sup>; <sup>1</sup>NIST Center for Neutron Research, NIST, Gaithersburg, Maryland; <sup>2</sup>Physics, UC Davis, Davis, California.

#### **GP3.04**

**Neutron Radiography and Tomography Study of Hydrided Zircaloy-4 Cladding Materials** Tyler Smith, Hassina Bilheux, Holly Ray, Jean-Christophe Bilheux and Yong Yan; Oak Ridge National Laboratory, Oak Ridge, Tennessee.

#### **GP3.05**

**Development of High Spatial Resolution at Engineering Diffractometer VULCAN** Alexandru D. Stoica<sup>1</sup>, Ke An<sup>1</sup>, Harley D. Skorpenske<sup>2</sup>, Rick Allen<sup>2</sup>, Wei Wu<sup>1</sup> and Matthew J. Frost<sup>2</sup>; <sup>1</sup>Chemical and Engineering Materials Division, ORNL, Oak Ridge, Tennessee; <sup>2</sup>Instrument and Source Division, ORNL, Oak Ridge, Tennessee.

#### **GP3.06**

**Temperature Effect on the Fatigue Behavior of Inconel Alloy 617 by In-Situ Neutron Diffraction Investigation** Bo-Han Wu<sup>1</sup>, E-Wen Huang<sup>1</sup>, Yu-lih Huang<sup>1</sup>, Wu Gong<sup>2</sup> and Stefanus Harjo<sup>2</sup>; <sup>1</sup>Chemical and Materials Engineering and Center for Neutron Beam Applications, National Central University, Taoyuan, N/A, Taiwan; <sup>2</sup>High Energy Accelerator Research Organization (KEK), Ibaraki, Japan.

#### **GP3.07**

**Different Compression Behaviors Between Zr<sub>64.13</sub>Cu<sub>15.75</sub>Ni<sub>10.12</sub>Al<sub>10</sub> and Zr<sub>59.63</sub>Cu<sub>15.75</sub>Ni<sub>14.62</sub>Al<sub>10</sub> Bulk Metallic Glasses** Gong Li, <sup>1</sup>The University of Tennessee, Knoxville, Tennessee; <sup>2</sup>Yanshan University, Qinhuangdao, China.

#### **GP3.08**

**The Effects of Microstructure and Heating Rate on Phase Transformation Behavior in a Dual Phase AHSS** Zhenzhen Yu<sup>1</sup>, John Vitek<sup>2</sup>, Ke An<sup>2</sup>, Zhili Feng<sup>2</sup>, Stan David<sup>2</sup> and Xun-Li Wang<sup>3</sup>; <sup>1</sup>Metallurgical and Materials Engineering, Colorado School of Mines, Golden, Colorado; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Physics & Materials Science, City University of Hong Kong, Kowloon, Hong Kong.

# H: Neutron Physics

\* Invited paper

SESSION HP1: Poster Session I: Neutron Physics  
Sunday Evening, June 1, 2014  
5:00 PM  
Summit II

## HP1.01

### Experimental Validation of the SNS Sample Activation

Calculator T. C. McClanahan, E. B. Iverson, F. X. Gallmeier and M. B. Smith; Neutronics Analysis, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## HP1.02

**The Ramsey Method – A Versatile Precision Technique in Neutron Physics** Florian M. Piegsa, Institute for Particle Physics, ETH Zurich, Zurich, Switzerland.

## HP1.03

**Strain Effect in FeN Multilayer Structure on GaAs Substrate** Xiaowei Zhang<sup>1,2</sup>, Nian Ji<sup>1,2</sup>, Valeria Lauter<sup>3</sup>, Hailemariam Ambaye<sup>3</sup> and Jian-Ping Wang<sup>1,2</sup>; <sup>1</sup>The Center for Micromagnetics and Information Technologies (MINT) & Electrical and Computer Engineering Department, University of Minnesota, Minneapolis, Minnesota; <sup>2</sup>School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota; <sup>3</sup>Neutron Science Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## HP1.04

**A New Experiment Towards Search for Neutron to Anti-Neutron Oscillation at the European Spallation Source** Matthew Frost, NNbarX Collaboration, The University of Tennessee-Knoxville, Knoxville, Tennessee.

SESSION H1: Nuclear/Particle/Astrophysics with Neutrons I

Session Chair: Scott Dewey  
Monday Morning, June 2, 2014  
Tennessee Ballroom C

## 10:15 AM \*H1.01

**Nuclear and Particle Physics with Neutrons at the Spallation Neutron Source** Nadia Fomin, University of Tennessee, Knoxville, Tennessee.

## 10:45 AM H1.02

**The NPDGamma Experiment: Using Neutrons to Probe the Nucleon-Nucleon Weak Interaction** Elise Tang, Physics and Astronomy, University of Kentucky, Lexington, Kentucky.

## 11:00 AM H1.03

**Search for the Neutron Electric Dipole Moment at the Paul Scherrer Institute** Florian M. Piegsa, Institute for Particle Physics, ETH Zurich, Zurich, Switzerland.

## 11:15 AM H1.04

**Measuring the Neutron Electric Dipole Moment at the SNS** Vince Cianciolo, Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

## 11:30 AM H1.05

**The Status of n3He Experiment at SNS** Irakli Garishvili, Physics, University of Tennessee, Knoxville, Tennessee.

## 11:45 AM H1.06

**Search for Time Reversal Invariance Violation in Xenon (Trex), Using a Polarized Epithermal Neutron Beam** Zhaowen Tang, Physics, Indiana University, Bloomington, Indiana.

## 12:00 PM H1.07

**The n-3He Incoherent Scattering Length Measured Using a Polarized Helium Cell Inside a Neutron Interferometer** Michael G. Huber<sup>1</sup>, Dmitry A. Pushin<sup>4</sup>, Fred E. Wietfeldt<sup>5</sup>, Chandra B. Shahi<sup>5</sup>, Muhammad Arif<sup>1</sup>, Wangchun C. Chen<sup>1,2</sup>, Thomas R. Gentile<sup>1</sup> and Timothy C. Black<sup>3</sup>; <sup>1</sup>NIST, Gaithersburg, Maryland; <sup>2</sup>University of Maryland, College Park, Maryland; <sup>3</sup>University of North Carolina-Wilmington, Wilmington, North Carolina; <sup>4</sup>University of Waterloo, Waterloo, Ontario, Canada; <sup>5</sup>Tulane University, New Orleans, Louisiana.

SESSION HP2: Poster Session II: Neutron Physics  
Monday Evening, June 2, 2014  
5:30 PM  
Summit II

## HP2.01

**Large Area Microchannel Plate Neutron Detectors for Neutron Scattering** Bruce Feller<sup>1</sup>, Richard A. Riedel<sup>2</sup>, Xiaodong Zhang<sup>3</sup>, Brian White<sup>1</sup> and Paul White<sup>1</sup>; <sup>1</sup>NOVA Scientific, Inc., Sturbridge, Massachusetts; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee; <sup>3</sup>Nuclear Engineering, University of Tennessee, Knoxville, Tennessee.

## HP2.02

**An Investigation of the Prompt Pulse Issue of the SNS HYSPEC Instrument** M. B. Smith, E. B. Iverson, F. X. Gallmeier, B. L. Winn and T. C. McClanahan; Oak Ridge National Laboratory, Knoxville, Tennessee.

SESSION H2: Nuclear/Particle/Astrophysics with Neutrons II

Session Chair: Zhaowen Tang  
Tuesday Afternoon, June 3, 2014  
Tennessee Ballroom C

## 1:45 PM \*H2.01

**Fundamental Physics with Neutrons at the NIST Center for Neutron Research** Scott Dewey, Neutron Physics, NIST, Gaithersburg, Maryland.

## 2:15 PM H2.02

**Quantum Information Processing Enabled Neutron Interferometry** Joachim Nsofini<sup>1,2</sup>, David Cory<sup>1,2</sup> and Dmitry Pushin<sup>1,2,3</sup>; <sup>1</sup>Physics, University of Waterloo, Waterloo, Ontario, Canada; <sup>2</sup>Physics Institute for Quantum Computing, University of Waterloo, Waterloo, Ontario, Canada; <sup>3</sup>D of Commerce, NIST, Gaithersburg, Maryland.

## 2:30 PM H2.03

**Development of In-Vacuum Thermally Controlled Neutron Interferometry** Ke Li<sup>1</sup>, Muhammad Arif<sup>2</sup>, Michael Huber<sup>2</sup>, Dmitry Pushin<sup>3</sup>, Vladimir Skavysh<sup>1</sup> and William M. Snow<sup>1</sup>; <sup>1</sup>Center for Exploration of Energy and Matter, Indiana University, Bloomington, Indiana; <sup>2</sup>National Institute of Standards and Technology, Gaithersburg, Maryland; <sup>3</sup>Institute for Quantum Computing, University of Waterloo, Waterloo, Ontario, Canada.

## 2:45 PM H2.04

**Quantum Correlations in a Noisy Neutron Interferometer** Christopher J. Wood<sup>1,2</sup>, David G. Cory<sup>3,2,4</sup>, Mohamed O. Abutaleb<sup>5</sup>, Michael G. Huber<sup>6</sup>, Dmitry A. Pushin<sup>1,2</sup> and Muhammad Arif<sup>6</sup>; <sup>1</sup>Physics and Astronomy, University of Waterloo, Waterloo, Ontario, Canada; <sup>2</sup>Institute for Quantum Computing, Waterloo, Ontario, Canada; <sup>3</sup>Chemistry, University of Waterloo, Waterloo, Ontario, Canada; <sup>4</sup>Perimeter Institute for Theoretical Physics, Waterloo, Ontario, Canada; <sup>5</sup>Massachusetts Institute of Technology, Cambridge, Massachusetts; <sup>6</sup>National Institute of Standards and Technology, Gaithersburg, Maryland.

## 3:00 PM H2.05

**Resonant Frequency Spin Rotator for the n3He Experiment** Christopher B. Hayes, Physics, University of Tennessee, Knoxville, Tennessee.

## 3:15 PM H2.06

**The n-3He Experiment – Target/Detector Chamber** Mark McCrea, Dept. of Physics and Astronomy, University of Manitoba, Winnipeg, Manitoba, Canada.

The Neutron Scattering Society of America is pleased to announce the 2014 recipients of its four major prizes.

**Prof. Sunil K. Sinha**

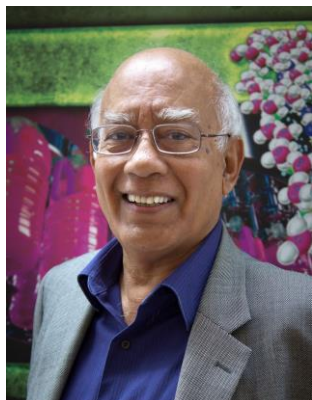
University of California San Diego

is the recipient of the

**2014 Clifford G. Shull Prize**

of the Neutron Scattering Society of America (NSSA) with the citation

*“In recognition of his deep and lasting experimental and theoretical contributions to the areas of Quantum Liquids and Solids, Superconductivity, Magnetism, Soft Condensed Matter, Confined and Adsorbed Liquids, Surfaces, and Neutron Scattering Techniques, together with his selfless service to the neutron scattering field as a whole”*



Prof. Sunil K. Sinha

The Neutron Scattering Society of America (NSSA) established the Clifford G. Shull Prize in Neutron Science to recognize *outstanding research in neutron science and leadership promoting the North American neutron scattering community*. The prize is named in honor of Prof. Clifford G. Shull, who received the Nobel Prize in 1994 with Prof. Bertram Brockhouse for seminal developments in the field of neutron science. The establishment of the prize was announced at the inaugural American Conference on Neutron Scattering (ACNS) in 2002.

The nominations were reviewed by a committee of experts in the field of neutron science and the NSSA is pleased to announce that the recipient of the 2014 Shull Prize is **Prof. Sunil K. Sinha**, University of California, San Diego. The prize and \$5000 honorarium will be awarded at the 2014 ACNS in Knoxville, TN, June 1-5, 2014 (<http://www.mrs.org/acns-2014>).

*“I feel deeply honored to be awarded the Clifford G. Shull Prize”* said Prof. Sunil K. Sinha. *“I have always been a great admirer of Cliff Shull and the pioneering work he did in our field, and I have always felt privileged to be a part of the neutron scattering community, united by a technique that has contributed so much to our understanding of condensed matter.”*





Most would take pride in a career achieving international recognition in a single niche of physics. Prof. Sinha's achievements produced international recognition over a broad range of topics in physics. The scope of Sinha's work ranges from theory to experiment, soft condensed matter to quantum solids, magnetic materials to superconductors, and from inelastic scattering to the myriad of elastic techniques. Prof. Sinha has demonstrated scientific versatility that is a fitting honor to Clifford Shull's legacy. He has pioneered applications of neutron scattering that have directly affected many neutron scattering research programs world-wide.

Prof. Sinha and his collaborators performed one of the earliest measurements of the phonon spectra of Quantum Crystals and his early neutron work demonstrated the coexistence of magnetism and superconductivity in  $\text{ErRh}_4\text{B}_4$ . Soon after the discovery of the high- $T_c$  cuprates, Sinha and collaborators discovered long-range antiferromagnetic order in the parent compounds  $\text{La}_2\text{CuO}_4$ ,  $\text{YBa}_2\text{Cu}_3\text{O}_6$ , and  $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ . Today it is recognized that the coexistence of magnetism and superconductivity is critical to our understanding of high- $T_c$  superconductivity.

Prof. Sinha's early neutron studies of two-dimensional adsorbed layers and their phase transitions include the first measurement of the power-law structure factor associated with pseudo-Bragg peaks of a 2-D solid. He analytically calculated the scattering function including finite size effects, and this is routinely used today. Prof. Sinha and collaborators carried out the first Small-Angle Neutron Scattering measurements that used methods they developed to analyze fractal structures, leading to the determination of the dimension and size of the fractal cluster. These methods are now widely emulated.

In 1988, Prof. Sinha published his seminal paper describing the theory of off specular x-ray and neutron scattering from rough surfaces and demonstrated innovative applications of the theory to studies of surface transitions in liquid and solid systems, multiple interfaces, thin films, and corrosion processes. Today, the off-specular scattering theory is a key tool in the extremely popular fields of x-ray and neutron reflectometry.

Prof. Sinha's employment record is as varied as his research program. The ability to perform great research at many different institutions, e.g., academia, industry and national labs, are an inspiration to all. Prof. Sinha received his PhD from Cambridge University in 1964. He was a Professor of Physics at Iowa State University from 1967-1974 and became a Senior Physicist at Argonne National Lab in 1975. From 1983 until 1995 Prof. Sinha was a Senior Research Associate at Exxon's Corporate Research Labs, where he played a critical role in the engagement of Exxon in neutron scattering research. In 1995 he became Associate Division Director for the Advanced Photon Source, and since 2001 has been a Distinguished Professor of Physics at the University of California San Diego.

## Dr. Jeffrey W. Lynn

National Institute of Standards and Technology

is the recipient of the

### 2014 Sustained Research Prize

of the Neutron Scattering Society of America (NSSA) with the citation

***“For seminal studies of the colossal magneto-resistance effect and profound contributions to our understanding of the interplay of magnetism and superconductivity.”***



Dr. Jeffrey W. Lynn

The Neutron Scattering Society of America (NSSA) established the Sustained Research Prize to recognize a *sustained contribution to a scientific subfield, or subfields, using neutron scattering techniques, or a sustained contribution to the development of neutron scattering techniques*. The primary consideration shall be an enduring impact on science. Preference shall be given to applicants whose work was carried out predominantly in North America.

The nominations were reviewed by a committee of experts in the fields to which neutron scattering contributes and the NSSA is pleased to announce that the 2014 recipient of the Sustained Research Prize is **Dr. Jeffrey W. Lynn** of the National Institute of Standards and Technology. The prize and \$2500 honorarium will be awarded at the 2014 ACNS in Knoxville, TN June 1-5, 2014 (<http://www.mrs.org/acns-2014/>).

Dr. Jeffrey W. Lynn has established an outstanding record of ground-breaking research on the physics of magnetic materials using neutron scattering. He began his career with insightful studies of ferromagnetic materials, both itinerant systems such as Fe, Ni and their alloys and systems where the electrons are more spatially localized such as transition metal oxides. This work helped to establish our current understanding of these materials, stimulating theoretical efforts and testing their boundaries. Throughout his career, Dr. Lynn refined and extended this early work to a variety of different systems, investigating how the static and dynamical aspects of magnetism are affected by the onset of different types of magnetic order. These later systems included manganese oxides, which display unusually large magnetoresistance, as well



as multiferroic materials, which simultaneously possess both ferromagnetic and ferroelectric order. Dr. Lynn's pioneering work on these materials profoundly affected both theoretical and computational studies.

Dr. Lynn has also made career-long contributions towards understanding the interplay between magnetism and superconductivity. He began this effort with his research on the rare earth molybdenum chalcogenides, where he helped to establish the role of magnetism as a driving force for other collective states, namely superconductivity. This led to more recent studies of cuprates and then pnictides, where he and his collaborators made seminal contributions to our knowledge of magnetic ordering in systems where magnetism and superconductivity exist in close proximity.

In addition to these major contributions to the understanding of magnetism and its role in many important phenomena, Dr. Lynn has served as a mentor to a long series of graduate and postdoctoral students, and many collaborators from other organizations, helping to establish a cadre of well-trained neutron scatterers. He also worked to help advance neutron scattering techniques by developing a new thermal triple axis spectrometer at the NIST Center for Neutron Research. This instrument combines many innovative features to provide unprecedented neutron intensity ideal for measurements of small samples, enabling many novel experimental studies.

Throughout his career Dr. Lynn has been an international leader and vocal advocate of the use of neutron scattering methods to answer fundamental questions in condensed matter physics. He exemplifies the characteristics for which this prize was established – sustained and significant contributions to both, techniques and their application to important scientific questions.

Dr. Lynn is a Fellow of the National Institute of Standards and Technology where he leads the Condensed Matter Physics team at the NIST Center for Neutron Research. He received his Ph.D. from Georgia Tech in 1974, performing neutron scattering measurements at Oak Ridge National Laboratory with Dr. Herbert Mook. He then took a post doc under the direction of Dr. Gen Shirane at Brookhaven National Laboratory. In 1976, he became a Professor at the University of Maryland and in 1992 joined NIST full time. Dr. Lynn has also held important advisory roles within the scientific community, including chair of the Division of Materials Physics of the American Physical Society and Program Co-Chair for the 2004 American Conference on Neutron Scattering. In 2011 President Obama conferred upon him the Presidential Rank Award of Distinguished Senior Professional. He is a fellow of both the American Physical Society and the NSSA.

## Dr. Emil Bozin

Brookhaven National Laboratory

is the recipient of the

### 2014 Science Prize

of the Neutron Scattering Society of America (NSSA) with the citation

***"For his discovery of broken symmetry local structures in exotic electronic materials, his elaboration of their nature and their importance to the material properties, in particular in PbTe, iridates, manganites, and cuprates"***



Dr. Emil Bozin

The Neutron Scattering Society of America (NSSA) established the Science Prize to recognize a *major scientific accomplishment or important scientific contribution within the last 5 years* using neutron scattering techniques. Nominees must be within 12 years of receiving their PhD degree. Preference shall be given to applicants whose work was carried out predominantly in North America.

The nominations were reviewed by a committee of experts in the scientific areas to which neutron scattering contributes, and the NSSA is pleased to announce that the 2014 recipient of the Science Prize is **Dr. Emil Bozin** of Brookhaven National Laboratory. The prize and \$2500 honorarium will be awarded at the 2014 ACNS in Knoxville, TN June 1-5, 2014 (<http://www.mrs.org/acns-2014/>).

Over the past 5 years, Dr. Bozin's application of the atomic pair distribution function (PDF) analysis to neutron powder diffraction data to study local and nanoscale structure in materials has led to key insights regarding the physics of complex oxide and chalcogenide electronic materials. The discovery of local distortions in rock-salt lead telluride on warming was published in Science in December 2010. Despite PbTe being extensively studied for more than a century, for example, for its exceptional thermoelectric properties, this result had not been previously known, as the effect is not visible in the average structure. This discovery had a



profound effect on the understanding of the heat capacity and the electronic band-gap. It is seminal in the sense that it has awakened an interest in the importance of characterizing anharmonic effects in crystals in general, and the value of searching for and studying local broken symmetry states in other materials.

Broken local symmetries in the form of charge and spin stripes are at the forefront of understanding high temperature superconductivity and Dr. Bozin's work has also had a large impact in that field, where the effects of broken local symmetries on the electronic structure have been suggested as an explanation for the mysterious pseudogap region of the cuprate phase diagram. His recent studies on related spinel systems like  $\text{Cu}(\text{Ir}_{1-x}\text{Cr}_x)_2\text{S}_4$  build on those results and show that these phenomena are widespread and not confined to a few exotic systems. Dr. Bozin's work showed that creative use of new developments in neutron diffraction and PDF can lead the way to deeper understanding of materials and their properties.

Dr. Bozin received his PhD in 2003 from Michigan State University, was Physics Lecturer at the Military Academy in Belgrade, Serbia, Postdoctoral Research Associate at Michigan State University, and Associate Research Scientist at Columbia University before joining Brookhaven National Laboratory in 2010. Dr. Bozin is currently Associate Scientist at Brookhaven National Laboratory.

## Dr. Kate A. Ross

Johns Hopkins University and  
NIST Center for Neutron Research

is the recipient of the

### 2014 Prize for Outstanding Student Research

of the Neutron Scattering Society of America (NSSA) with the citation

***"For seminal neutron scattering studies of exotic ground states, ground state selection, and spin excitations in XY Pyrochlore Magnets"***



The Neutron Scattering Society of America (NSSA) established the Prize for Outstanding Student Research to recognize *outstanding accomplishments in the general area of neutron scattering by graduate or undergraduate students who have performed much of their work at North American neutron facilities*. Nominees must be either current graduate students or scientists within two years of receiving their PhD.

Dr. Kate A. Ross

The nominations were reviewed by a committee of experts in the field of neutron science and the NSSA is pleased to announce that the recipient of the 2014 Prize for Outstanding Student Research is **Dr. Kate A. Ross** of the Johns Hopkins University and NIST Center for Neutron Research. The prize and \$1000 honorarium will be awarded at the ACNS in Knoxville, TN June 1-5, 2014 (<http://www.mrs.org/acns-2014/>).

Pyrochlore magnets have been a playground for the physics of exotic ground states, as many different magnetic ions can be made to decorate the pyrochlore lattice - a network of corner-sharing tetrahedra and one of the defining architectures supporting geometrical frustration in three dimensions. During her graduate studies at McMaster University, Dr. Ross carried out a series of sophisticated neutron scattering experiments on two such materials,  $\text{Yb}_2\text{Ti}_2\text{O}_7$  and  $\text{Er}_2\text{Ti}_2\text{O}_7$ , wherein the local symmetry of the rare-earth moments is planar, or XY-like. This local symmetry implies that quantum effects are extreme, due to effective  $S=1/2$  magnetic moments, in these two materials.



Working at dilution refrigerator temperatures and in high magnetic fields at the NIST Center for Neutron Research, Dr. Ross acquired comprehensive inelastic neutron scattering data, which were used to unambiguously determine the full spin Hamiltonian for these magnets, based on anisotropic exchange. This work provided a natural explanation for a quantum spin ice ground state in  $\text{Yb}_2\text{Ti}_2\text{O}_7$ , and for ground state selection *via* an order-by-disorder mechanism in  $\text{Er}_2\text{Ti}_2\text{O}_7$ . She also carried out systematic powder neutron diffraction measurements at the Lujan Neutron Scattering Center, which identified the microscopic source of weak sample-to-sample variability in  $\text{Yb}_2\text{Ti}_2\text{O}_7$ .

Dr. Ross graduated from McMaster University in September of 2012, and is currently a postdoctoral fellow in the Institute for Quantum Matter and Department of Physics and Astronomy at Johns Hopkins University, as well as at the NIST Center for Neutron Research. Her current interests include new magnetic materials, as well as technique development and extreme sample environments, particularly as they pertain to the elucidation of quantum physics in new materials.