

SNAP/COMPRES 2008

A Joint Meeting Exploring Opportunities for Scattering using Neutrons and HE X-rays

Spallation Neutrons and Pressure
5th Annual Meeting

April 13-15, 2008
Oak Ridge, Tennessee

Saturday, April 12 – Sunday, April 13, 2008

Arrival and Check-in

The Oak Ridge Comfort Inn
433 S. Rutgers Avenue
Oak Ridge, Tennessee 37830
Tel: 865-481-8200

(Please pick up your meeting packet at the front desk when you check in).

Sunday, April 13, 2008 “Meet & Greet” Informal Gathering

5:00 – 9:00pm *Jalisco Mexican Restaurant*
(Walking Directions in Meeting Packet)

Monday, April 14, 2008, bldg 8600, rm 156

8:00am **BADGING (See Instructions on Greetings page)**

INTRODUCTIONS: SNS, SING, SNAP UPDATES – Chair: John Parise

9:00 – 9:05am	Welcome John B. Parise, Stony Brook University
9:05 – 9:20am	Overall SNS Status Ken Herwig, Oak Ridge National Laboratory
9:20 – 9:35am	SING → SNS → SNAP Barbara Thibadeau, Oak Ridge National Laboratory
9:35 – 9: 50am	Beamline Status Specifics Christopher A. Tulk, Oak Ridge National Laboratory
9:50 – 10:00am	Discussion
10:00 – 10:10am	COMPRES and User Facilities for Mineral Physics Research Robert C. Liebermann, COMPRES
10:10 – 10:15am	Discussion

Emerging Capabilities for Neutron and High Energy X-ray Research:

Chair – Chris Tulk

10:15 – 10:35am **Changes in the Structure of MgO-SiO₂ Glasses with Pressure: In Situ Neutron Diffraction Results**
Martin Wilding, University of Wales, Aberystwyth

10:35 – 10:40am **Discussion**

10:40 – 10:55am ***BREAK***

10:55 – 11:15am **High Pressure High Temperature**
Stefan Klotz, IMPMC

11:15 – 11:20am **Discussion**

11:20 – 11:40am **Complementing IXS and LH-DAC Experiments with DFPT Modeling**
Bjoern Winkler, Universitaet Frankfurt

11:40 – 11:45am **Discussion**

11:45 – 11:55pm **IMAGINE Quasi-Laue Diffractometer at the HFIR**
Bryan Chakoumakos, ORNL

11:55 – 12:00pm **Discussion**

12:00 – 1:00pm ***LUNCH***

High Pressure Single Crystal Techniques: Chair – Chris Tulk

1:00 – 1:20pm **Software Requirements for Single Crystal Diffraction**
Ross Angel, Virginia Tech

1:20 – 1:25pm **Discussion**

1:25 – 1:45pm **Data Visualization and Reduction for Single-Crystal Diffraction at the ILL**
Garry McIntyre, Institut Laue-Langevin

1:45 – 1:50pm **Discussion**

1:50 – 2:10pm **Studying High-pressure Transformations of Possible Light-element Phases in the Core and Development of Novel Single-crystal Diffraction Techniques for High-pressure Crystallography**
Przemek Dera, University of Chicago

2:10 – 2:15pm **Discussion**

2:15 – 2:30pm **The Structural Diversity of Sodium**
Eugene Gregoryanz, University of Edinburgh

2:30 – 2:35pm **Discussion**

Facilities Updates:

- 2:35 – 2:50pm** **Update on JPARC**
Wataru (Sho) Utsumi, Japan Atomic Energy Agency
- 2:50 – 2:55pm** **Discussion**
- 2:55 – 3:10pm** **Plans and Updates on the High-pressure Beamline Project in Japan**
Hiroyuki Kagi, University of Tokyo
- 3:10 – 3:15pm** **Discussion**
- 3:15 – 3:30pm** **Plans for High Energy Scattering at X17A, NSLS**
Lars Ehm, Mineral Physics Institute, Stony Brook University
- 3:30 – 3:35pm** **Discussion**
- 3:35 – 3:45pm** ***BREAK***

SHORT PRESENTATIONS – Hydrogen in Minerals and Ices:

Chair – John Parise

- 3:45 – 3:55pm** **Nucleation and Growth of Ice XI**
Hiroshi Fukazawa, Japanese Atomic Energy Agency
- 3:55 – 4:00pm** **Discussion**
- 4:00 – 4:15pm** **Molecular Dynamic Simulations at HP of Clathrate Hydrate Systems**
Dennis Klug, National Research Council of Canada
- 4:15 – 4:20pm** **Discussion**
- 4:20 – 4:35pm** **High Energy X-ray Scattering Studies at HP of Clathrate Hydrate Systems**
Chris Tulk, Oak Ridge National Laboratory
- 4:35 – 4:40pm** **Discussion**
- 4:40 – 4:55pm** **Joint X-N Studies of Hydrogenous Materials**
John Loveday, University of Edinburgh
- 4:55 – 5:00pm** **Discussion**
- 5:00 – 5:10pm** **High Energy X-ray Diffraction Studies of Filled Ice (Ar-H₂O at High Pressure)**
Ling Yang, Oak Ridge National Laboratory
- 5:10 – 5:15pm** **Discussion**
- 7:00 – 9:00pm** ***DINNER: Peerless Steakhouse***

Tuesday, April 15, 2008, bldg 8600, rm 156

8:00 – 8:30am Coffee and Mingle

Novel Hardware – Novel Science: Chair – Robert Liebermann, COMPRES

- 8:30 – 8:50am Temperature at Pressure: Novel Studies**
David Dobson, University College London
- 8:50 – 8:55am Discussion**
- 8:55 – 9:15am Density Measurement at High-Pressure and Applications to the Deep Earth**
David Walker, Columbia University
- 9:15 – 9:20am Discussion**
- 9:20 – 9:35am Topaz Update**
Christina Hoffman, Oak Ridge National Laboratory
- 9:35 – 9:40am Discussion**
- 9:40 – 9:55am Multi-anvils PE Cell for Ex Situ and Angle X-ray Diffraction Studies**
Yann LeGodec, IMPMC
- 9:55 – 10:00am Discussion**
- 10:00 – 10:15pm Inelastic Neutron Scattering Studies of Adsorbed Water on Oxide Nanoparticles**
Nancy Ross, Virginia Tech
- 10:15 – 10:20pm Discussion**
- 10:20 – 10:30am BREAK*

EMERGING OPPORTUNITIES I: Glasses, Melts, Liquids and Networks:
Chair – Rus Hemley

- 10:30 – 10:50am Network and Molecular Glasses at High Pressure**
Chris Benmore, Argonne National Laboratory
- 10:50 – 10:55am Discussion**
- 10:55 – 11:15am Structure Measurements at Extreme Temperatures and Under Non-equilibrium Conditions**
Richard Weber, Materials Development, Inc.
- 11:15 – 11:20am Discussion**
- 11:20 – 11:35am High Energy XRD Studies Under High Pressure for Metallic Glasses and Other Amorphous Materials**
Haozhe Liu, Harbin Institute of Technology, China
- 11:35 – 11:40am Discussion**

- 11:40 – 11:55pm** **High-pressure Studies of Novel Perovskite Compounds**
Changqing Jin, Inst of Physics, Chinese Academy of Sciences
- 11:55 – 12:00pm** **Discussion**
- 12:00 - 12:10 pm** **High Energy X-ray Diffraction Studies of High Pressure Crystalline and Amorphous Germanium Based Clathrates**
Anotonio Moreira Dos Santos, Oak Ridge National Laboratory
- 12:10 – 12:15 pm** **Discussion**
- 12:15 – 12:25 pm** **Compressed CaSiO₃ Glass**
Cathy Tarabrella, Stony Brook University
- 12:25 – 12:30 am** **Discussion**
- 12:30 – 1:30 pm* *LUNCH*

EMERGING OPPORTUNITIES II: Nanoparticles and Networks:
Chair – John Parise

- 1:30 – 1:45pm** **What it Takes to Make the Best PDF Measurements with High Energy X-rays and Area Detectors**
Peter Chupas, Argonne National Laboratory
- 1:45 – 1:50pm** **Discussion**
- 1:50 – 2:05pm** **Structural Studies of Functional Coordination Framework Materials**
Karena Chapman, Argonne National Laboratory
- 2:05 – 2:10pm** **Discussion**
- 2:10– 2:20pm** **Pressure-Induced Polymerization of Diiodobutadiyne in Assembled Co-Crystals**
Chris Wilhelm, Stony Brook University
- 2:20 – 2:25pm** **Discussion**
- 2:25 – 2:40pm** **High Pressure Study of Magnetization of Organometallic Complexes**
John Tse, University of Saskatchewan
- 2:40 – 2:45pm** **Discussion**
- 2:45 – 3:15pm** **Closing Remarks**
- 3:15 – 3:30pm* *BREAK*

FACILITY TOURS: Chris Tulk