

**2010 IUCr Meeting of the Commission on High Pressure:
Structure under Extreme Conditions of Pressure and Temperature**

September 19-23, 2010 Gatlinburg, TN

In 1996, the Commission on High Pressure of the International Union of Crystallography (IUCr) was established to represent and support high-pressure crystallography. The subsequent preceding decade had seen an extraordinary growth in the range and quality of high-pressure diffraction studies — particularly using powder methods — on both synchrotron and neutron sources. This had been stimulated by the power of modern sources, and by major developments in detectors and high-pressure technology. The High-Pressure Commission has maintained a high level of activity from its inception, in particular with organizing a series of international workshops held most recently in Oxford, United Kingdom; Harbin, China; Saskatoon, Canada and Florence, Italy. This meeting is a continuation in this series.

Sunday, September 19

6:00 pm- 8:00 pm Check-in and Welcome Reception, Airport Hilton Hotel

7:00 pm Chris Tulk, Oak Ridge National Laboratory: Meeting and Tour Overview

Monday, September 20

9:00 am Load buses and travel to Oak Ridge National Laboratory

10:00 am ORNL tour

12:30 pm Working Lunch

2:00 pm Load buses and travel to Park Vista Hotel in Gatlinburg

6:30 pm Instrument Overview of High Flux Isotope Reactor (HFIR) Instruments: Poster Session and Reception

Tuesday, September 21

9:00 am Welcome / Introductory comments by Przemyslaw Dera and Chris Tulk

9:30 am Plenary lecture -John Parise (Stony Brook University, Brookhaven National Laboratory)
"Personal reflections on the past, present and future of high pressure scattering studies"

10:30 am Break

11:00 am - **Crystal Structures and Phase Transitions**

3:00 pm Session chair: Lars Ehm (Stony Brook University, National Synchrotron Light Source)

11:00 am Invited speaker: Maik Lang (University of Michigan)
"Coupling high-pressure cells with large ion accelerators: Solids at extreme conditions"

11:30 am Lauren Borkowski (Stony Brook University)
"High pressure behavior of $[\text{HN}(\text{CH}_2\text{CH}_2)_3\text{NH}][\text{V}_{2\text{V}4\text{IV}}\text{O}_{14}] \cdot \text{H}_2\text{O}$ "

11:50 am Atsushi Kyono (Carnegie Institution of Washington)
"High-pressure single-crystal X-ray diffraction study of phase transformation in chromite"

12:10 pm Souleymane Omar Diallo (Oak Ridge National Laboratory)
"Quest for Bose-Einstein condensate in solid ^4He "

12:30 pm Lunch

- 1:30 pm Malcolm Guthrie (Carnegie Institution of Washington)
"Proton disorder in ice VII up to 24 GPa"
- 2:00 pm Ingo Loa (University of Edinburgh)
"Truly complex elemental crystal structures: Barium"
- 2:30 pm Invited speaker: Eugene Gregoryanz (University of Edinburgh)
"Simple systems at extreme conditions"
- 3:00 pm Break
- 3:30 pm - **Biological Materials**
5:00 pm Session chair: Francesca Fabbiani (Georg-August-Universität Göttingen)
- 3:30 pm Invited speaker: Judith Peters (Institut de Biologie Structurale)
"Effect of pressure on the dynamics of proteins"
- 4:00 pm Invited speaker: Chae Un Kim (Cornell High Energy Synchrotron Source)
"High pressure study on water inside protein crystals"
- 4:30 pm Francesca Fabbiani (Georg-August-Universität Göttingen)
"Exploring disorder and conformational flexibility in vitamin B12 at high pressure"
- 7:00 pm - Satellite meeting: Deep Carbon Observatory/Sloan Foundation-sponsored
8:30 pm roundtable discussion of future large-scale instrumentation needs
(Open to all meeting participants)

Wednesday, September 22

- 8:30 am - **Materials Science**
9:40 am Session chair: Haozhe Liu (Harbin Institute of Technology)
- 8:30 am Invited speaker: Oleksandr Kurakevych (IMPIC, University P&M Curie)
"High-pressure route to superhard boron-rich solids"
- 9:00 am Helen Maynard-Casely (University of Edinburgh)
"Crystal engineering with pressure – applications for energetic materials"
- 9:20 am Wilson Crichton (European Synchrotron Radiation Facility)
"New structures in AX₂, AX₃ and ABX₄ systems; exploration of systematic relationships between type-structures"
- 9:40 am - **Techniques for High-Pressure Studies**
12:20 pm Session chair: Chris Tulk (Oak Ridge National Laboratory)
- 9:40 am Invited speaker: Hiroyuki Kagi (University of Tokyo)
"High-pressure beamline (PLANET) at the spallation neutron source in J-PARC"

- 10:10 am Break
- 10:40 am Invited speaker: Vitali Prakapenka (University of Chicago)
"On-line combination of optical and synchrotron X-ray techniques for high pressure research"
- 11:10 am Invited speaker: Timothy Jenkins (NIST Center for Neutron Research)
"High-pressure research at NCNR"
- 11:40 am Jörg Wiesmann (Incoatec GmbH)
"Progress in Using Short Wavelength Radiation for Chemical and High-Pressure Crystallography"
- 12:00 am Chris Tulk (Oak Ridge National Laboratory)
"The SNAP high-pressure diffractometer at the Spallation Neutron Source"
- 12:20 pm Instrument Overview of Spallation Neutron Source (SNS) Instruments I: Poster Session and Lunch
- 1:20 pm - **Simple Organic Systems**
2:50 pm Session chair: Maddury Somayazulu (Carnegie Institution of Washington)
- 1:20 pm Invited speaker: Frederic Datchi (CNRS and Université Paris 6)
"Structure of molecular CO₂ at high pressures and temperatures"
- 1:50 pm Invited speaker: Timothy Strobel (Carnegie Institution of Washington)
"Novel hydrogen-rich molecular solids at high pressure"
- 2:20 pm Invited speaker: Kamil Dziubek (Adam Mickiewicz University)
"Pressure-induced conformational changes in molecular crystals"
- 2:50 pm Break
- 3:20 pm - **Amorphous, liquid, non-crystalline and nanocrystalline systems**
4:50 pm Session chair: Yoshinori Katayama (Japan Atomic Energy Agency)
- 3:20 pm Invited speaker: Stanimir Bonev (Lawrence Livermore National Laboratory and Dalhousie University)
"Dense nitrogen: from molecular liquid to polymeric liquid to polymeric solid"
- 3:50 pm Invited speaker: Tomoko Sato (Institute for Solid State Physics, University of Tokyo)
"High-pressure behavior of SiO₂ glass"
- 4:20 pm Yoshinori Katayama (Japan Atomic Energy Agency)
"Structure of water under high pressure and high temperature"

- 5:45 pm Travel to the Aquarium of the Smokies
- 6:00 pm - Free time at the Aquarium of the Smokies
7:00 pm
- 7:00 pm Conference Dinner at the Aquarium of the Smokies
Keynote Speaker: Dean Myles, Director, Neutron Scattering Science Division

Thursday, September 23

8:30 am - **Geosciences and Planetary Sciences**

10:00 am Session chair: Barbara Lavina (HiPSEC-UNLV)

8:30 am Invited speaker: Nadege Hilairet (GSE-CARS)

“HP-HT deformation experiments in large volume press coupled with synchrotron monochromatic X-rays: olivine flow mechanisms in the earth’s mantle”

9:00 am Invited speaker: Simon Redfern (University of Cambridge)

“Structure, microstructure, elasticity and anelasticity in geomaterials under deep Earth conditions”

9:30 am Barbara Lavina (HiPSEC-UNLV)

“Structure factors from synchrotron single-crystal diffraction at high pressure”

10:00 am Break

10:30 am - **Theory and Computation**

12:10 pm Session chair: John Tse (University of Saskatchewan)

10:30 am Invited speaker: Dennis Klug (National Research Council of Canada)

“Structures and properties predictions of simple solids by metadynamics, random search and genetic algorithm methods”

11:00 am Konstantin Khishchenko (Russian Academy of Sciences)

“Thermodynamic modeling of structural transformations of metals at high pressures and temperatures”

11:20 am Yansun Yao (National Research Council of Canada)

“Temperature-dependent phase transitions of dense Mg and Ca”

11:40 am Invited speaker: Vladimir Stegailov (Russian Academy of Sciences)

“Premelting of iron: Implications for high-pressure melting curve measurements”

12:10 pm Instrument Overview of Spallation Neutron Source (SNS) Instruments II: Poster Session and Lunch

- 1:10 pm - **Chemistry**
3:50 pm Session chair: Kamil Dziubek (Adam Mickiewicz University)
- 1:10 pm Kenichi Takemura (NIMS)
"High-pressure structures of Na-Au intermetallic compounds"
- 1:30 pm Invited speaker: Ashkan Salamat (European Synchrotron Radiation Facility)
"High-pressure syntheses of novel high-density C-N-H materials from molecular precursors"
- 2:00 pm Invited speaker: Maddury Somayazulu (Carnegie Institution of Washington)
"Chemical bonding and compound formation in Xe-H₂, Xe-Br₂ and Xe-Cl₂ at high pressures and temperatures"
- 2:30 pm Break
- 3:00 pm John Lazarz (University of Chicago)
"Successive, pressure-induced development of bonding in NiAs type compounds and polymorphism of NiP"
- 3:20 pm Invited speaker: Choong-Shik Yoo (Washington State University)
"Synthesis of monolithic high energy density extended solids at extreme conditions"
- 3:50 pm - **Magnetic and Electronic Phenomena at High Pressure**
4:40 pm Session chair: Ingo Loa (University of Edinburgh)
- 3:50 pm Invited speaker: Naohisa Hirao (JASRI/SPring-8)
"Energy-domain synchrotron radiation Mössbauer spectroscopy in the multimegabar pressure range and its application to Fe"
- 4:20 pm Antonio Moreira dos Santos (Oak Ridge National Laboratory)
"Magnetic transitions in CoO"
- 4:40 pm Invited speaker: Serena Margadonna (University of Edinburgh)
"Pressure evolution of the low-temperature crystal structure of the FeSe superconductor"
- 5:10 pm Closing remarks