CDAC

CARNEGIE/DOE ALLIANCE CENTER

A Center of Excellence for
High Pressure Science and Technology
Supported by the Stewardship Science
Academic Alliances Program of DOE/NNSA

Annual Report
2011-2012

Russell J. Hemley, *Director*
Stephen A. Gramsch, *Coordinator*
Morgan Phillips Hoople, *Administrator*

NNSA
CARNEGIE INSTITUTION FOR SCIENCE

Carnegie/DOE Alliance Center (CDAC):
A CENTER OF EXCELLENCE FOR HIGH PRESSURE SCIENCE AND TECHNOLOGY

2009-2010 ANNUAL REPORT

On the Cover

Cockwise from top: 1) Brilliant-cut anvil prepared from diamond material grown by the CVD process at Carnegie. 2) CDAC graduate students Eloisa Zapeda, Jane Kanitpanyacharoen and Pamela Kaercher from UC-Berkeley prepare a resistively heated diamond anvil cell for radial diffraction measurements at HPCAT. 3) Four-probe configuration for electrical resistance measurements on a sample of semimetallic carbon disulfide at 10 GPa. 4) An optical cell developed by CDAC graduate student Kimberly Adams at Northwestern University for IR measurements on light hydrocarbons consists of 1 mm culets polished onto sapphire spheres and a gold gasket. 5) Diamond windows 3.0 mm in diameter and 0.5 mm thick, fabricated at Carnegie from CVD-grown diamond material, to be used for small-angle x-ray scattering measurements.

1. OVERVIEW

Since 2003, the Carnegie-DOE Alliance Center (CDAC) has served the nation as the DOE/NNSA's academic center for basic materials research in support of stockpile stewardship. Managed at the Carnegie Institution in Washington, D.C., as part of NNSA's Stockpile Stewardship Academic Alliances (SSAA) Program, CDAC builds on the institution's long record of advancing fundamental science at the frontiers of knowledge, which is vital to the security of our nation.[1, 2]

The mission of the Center is to expand understanding materials behavior at extreme pressure-temperature (*P-T*) conditions, to develop new experimental methods and facilities needed to advance high *P-T* materials science, and to support the education and training of next generation scientists in the field (Fig. 1). To accomplish these goals, CDAC maintains a coordinated program of basic research, educational outreach and technique development that contributes to the continued success of modern stockpile stewardship.

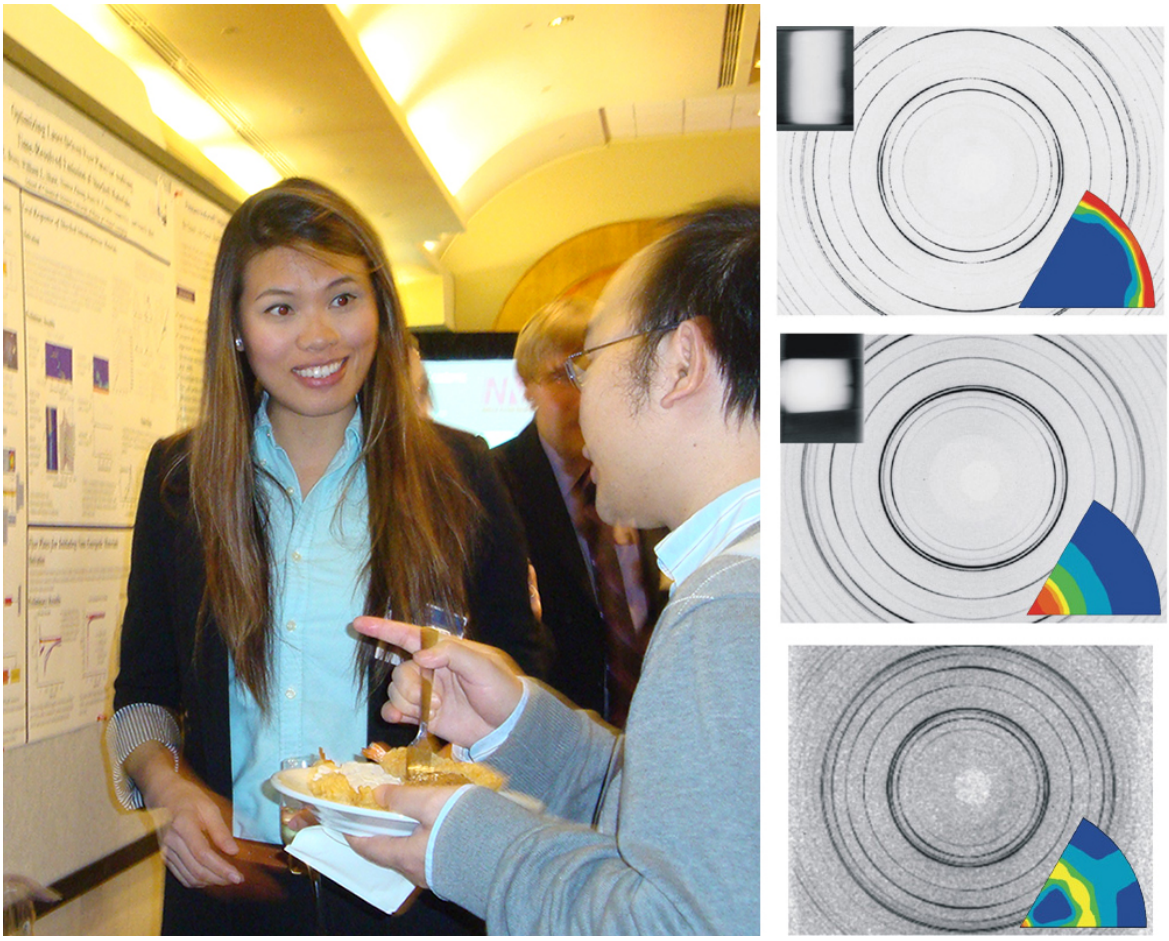


Figure 1. *CDAC investments in student education and training are benefiting graduate students at Academic Partner institutions, such as* ***Jane Kanitpanyacharoen (UC-Berkeley)****, shown here discussing her work with* ***HPCAT*** *beamline scientist* ***Yuming Xaio*** *at the 2012 SSAA Symposium. Jane and her fellow CDAC graduate students have carried out much of their dissertation research at* ***HPCAT****, a CDAC-supported facility at the* ***APS****. Jane's work on the texture evolution of hexagonal metals Zr and Hf with pressure (right) has benefitted significantly from the brilliance of the x-ray source at the APS. Along with advanced instrumentation and expert assistance available at HPCAT, CDAC students obtain state-of-the-art data using x-ray and associated techniques.*

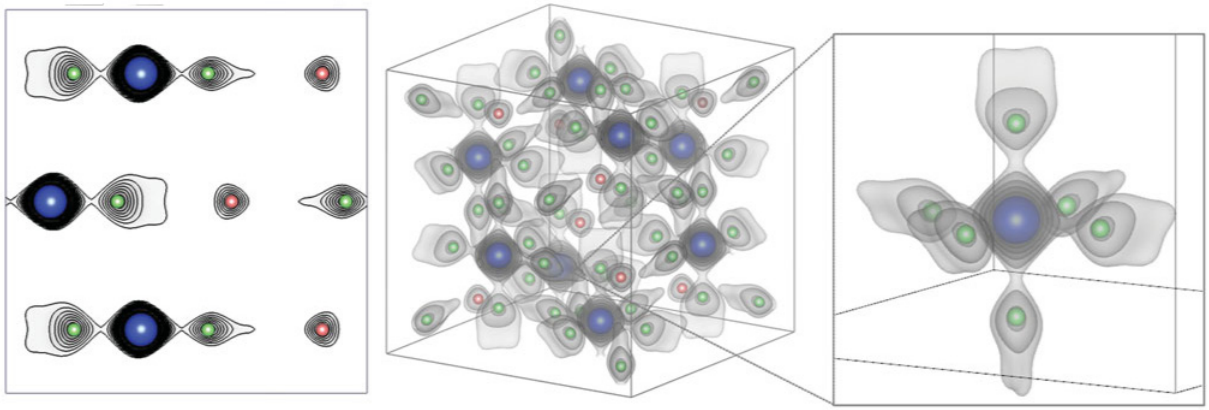


Figure 2. *Electron density distribution in silicon at 12.4 GPa. Left, [110] projection showing host lattice positions (blue) and precursor lattice positions (red and green). Center, three-dimensional view of the electron density distribution. Right, local view of the electron density distribution around a host lattice position showing the S_4 symmetry of the site.*[11]

1.1 CDAC at 10 Years

During the 10 years that the Center has been operating, we have significantly broadened our scientific scope, both by adding new partners and by facilitating the work of graduate students to explore new areas of high *P-T* materials science. From an initial group of six Academic Partners, we have now grown to 17 Academic Partners as well as a number of Laboratory Partners from the high pressure research groups of all three NNSA Labs. The variety of materials investigated by CDAC personnel now encompasses high *P-T* structural, optical, electronic and magnetic phenomena in a wide range of materials including metals, alloys, dense oxides, molecular systems and polymers, and composites and explosives; materials are studied in bulk, at surfaces and at interfaces (Fig. 2).

CDAC is managed at Carnegie by **Russell Hemley** (Director), **Stephen Gramsch** (Coordinator) and **Morgan Phillips Hoople** (Administrator). CDAC facilities at Carnegie are supported by Research Scientists **Maddury Somayazulu** and **Chang-sheng Zha**, and are made available to graduate students and collaborators from across the Center.

CDAC personnel take advantage of the capabilities – and support for NNSA science – available at DOE Office of Science (SC) user facilities at the **Advanced Photon Source** (**APS**, Fig. 3), **Argonne National Laboratory** (**ANL**), the **National Synchrotron Light Source** (**NSLS**), **Brookhaven National Laboratory** (**BNL**) and the **Lujan Neutron Scattering Center** at **LANSCE** at **Los Alamos National Laboratory** (**LANL**). Our support for these SC national user facilities

Figure 3. *U.S. Department of Energy Secretary* ***Steven Chu*** *visited* ***HPCAT*** *on Friday, June 3, 2011.* ***Russell Hemley*** *presented an overview of* ***HPCAT*** *and led the tour for the delegation, which included* ***University of Chicago*** *President* ***Robert J. Zimmer*** *and ANL Director* ***Eric Isaacs****.*

highlights one of the goals of our Center, and that is to promote partnerships between DOE/SC and DOE/NNSA programs.

During 2011-2012, CDAC supported graduate student education and training at 17 Academic Partner institutions, which represent many of the leading high pressure research groups in the United States (Box 1). Academic Partners in CDAC provide education and training for supported graduate students at the home institution, while CDAC provides many opportunities for interaction with graduate students from other groups as well as scientists from the NNSA Laboratories. The Center also makes beam time available at CDAC-supported user facilities at the **APS** (HPCAT, Fig. 4) and the **NSLS** (**U2A**). This arrangement has been remarkably productive (Box 2), but statistics tell only part of the story. In fact, the strength of the Center has been our efforts toward merging the various aspects of the high pressure community in this country (academic community, national laboratory groups, and specialized user facilities) to move the field forward while addressing NNSA needs in Stewardship Science.

Box 1. CDAC Academic Partners for 2011-2012.

- **David Cahill** (University of Illinois)
- **Dana Dlott** (University of Illinois)
- **Thomas Duffy** (Princeton University)
- **Rodney Ewing** (University of Michigan)
- **Brent Fultz** (California Institute of Technology)
- **Steven Jacobsen** (Northwestern University)
- **Abby Kavner** (University of California – Los Angeles)
- **Kanani Lee** (Yale University)
- **Jie Li** (University of Michigan)
- **Jung-Fu Lin** (University of Texas at Austin)
- **Wendy Mao** (Stanford University)
- **Wendy Panero** (Ohio State University)
- **Surendra Saxena** (Florida International University)
- **James Schilling** (Washington University at St. Louis)
- **Yogesh Vohra** (University of Alabama – Birmingham)
- **Hans-Rudolf Wenk** (University of California – Berkeley)
- **Jeffrey Yarger** (Arizona State University)

Joining the CDAC Academic Partners is a group of scientists from the high pressure research groups at the NNSA Labs. These Laboratory Partners serve on the CDAC Steering Committee, providing valuable input and expertise on the structure of the CDAC scientific program. In addition, the Laboratory Partners represent points of contact at the NNSA Labs for CDAC graduate students and Academic Partners. Laboratory Partners also benefit from beam time at HPCAT and U2A for their research projects, both programmatic and individual. At CDAC outreach events such as our Summer School and Winter Workshop, along with annual SSAA Symposia, NNSA Laboratory Partners interact directly with graduate students. This type of interaction has been invaluable in the career planning of CDAC students. CDAC graduate students have been introduced to postdoctoral opportunities in the NNSA Labs, and two of our students have accepted postdoctoral appointments in the past year. Moving forward, we continue to send our graduate students to the NNSA Labs each year, with both students and the Labs benefitting from the diverse scientific environment that characterizes the CDAC program.

At the beginning of the Center, we set out to make progress in the coordination of static and dynamic compression methods for stockpile stewardship. During our second five-year grant period, we provided beam time first at **NSLS-U2A** (to **Sandia National Laboratories, SNL**) and later at

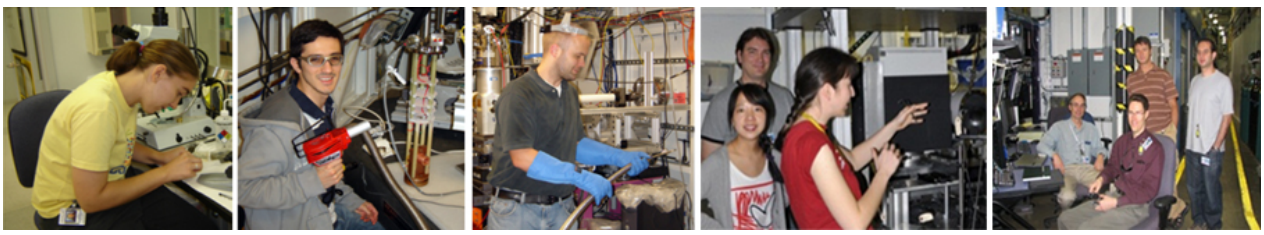


Figure 4. *CDAC users at* ***HPCAT.***

HPCAT (to **Washington State University-Institute for Shock Physics**) for the first synchrotron measurements of dynamic compression processes. Both experiments were extremely successful, and laid the groundwork for the formation if the Dynamic Compression Sector at the **APS** (DCS@APS), which is now in the final planning stages, with construction to begin in 2013. With the fruitful interactions taking place between DCS@APS and HPCAT, our understanding of materials behavior will advance into new *P-T* regimes, to the substantial benefit of NNSA science. This effort is also enhancing fundamental science at facilities such as Z (**SNL**) and NIF (**Lawrence Livermore National Laboratory, LLNL**), smaller laser shock platforms, and future facilities in the planning stages.

Box 2. CDAC Statistic for 2011-2012.

- Publications for 2011-2012 – **278**
  - *PNAS* – **12**
  - *Science* – **4**
  - *Nature* – **2**
  - *Physical Review Letters* – **23**
- Presentations for 2011-2012 – **342**
- Student Publications for 2011-2012 – **104**
- Student Presentations for 2011-2012 – **59**
- Collaborators for 2011-2012 – **747** from **162** Institutions
- Presentations at AGU 2011 – **68**
- Presentations at AGU 2012 – **62**
- PhDs Supported – **28**
- CDAC Students 2011-2012 – **35**
- Students & Post-docs to National Labs in 2011-2012 – **4**

The High Pressure Synergetic Center (HPSynC) at the APS is poised to make key contributions in this effort as well. Over the past four years, HPSynC has been an important resource in building the high pressure research community through a dual program of technique development and scientific outreach. The impact of the extreme conditions research spearheaded by HPCAT consistently raises opportunities for additional measurement and imaging experiments that are best addressed at other, more specialized beamlines at the **APS** that can be adapted for high pressure work. The technical capabilities of other **APS** beamlines has now increased the profile of extreme conditions research at the **APS**. HPSynC is responsible for several collaborations and important new experimental methods that will be significant in addressing problems of relevance to the NNSA mission, particularly through the coordination of scientific and technical development activities between HPCAT and DCS.

This report outlines the progress of the Carnegie-DOE Alliance Center, including its Academic and Laboratory Partners during 2011-2012. Research of Laboratory Partners done outside of CDAC-supported facilities is not covered.

1.2 Highlights from 2011-2012

Outreach and Training

- During 2011-2012, 17 Academic Partners supervised the education and training of 35 graduate students and postdoctoral fellows. During this time period, 10 CDAC-supported students received the PhD degree, working on projects in the area of high *P-T* materials science.

- CDAC graduate student **Joshua Townsend** (**Northwestern**) was the recipient of the 2012 E.H. Kraus Crystallographic Research Grant from the Mineralogical Society of America for his proposal entitled, "Extra-solar planetary mineralogy: The role of H_2O in crystal structures." The award will support his research in the area of high-pressure mineral and materials physics.

- Former CDAC student **Lowell Miyagi** has accepted a tenure-track faculty position at the **University of Utah**. Lowell was a student of CDAC Partner **Hans-Rudolf Wenk** at **Berkeley**, where he studied deformation of materials at high *P-T* conditions. After receiving his Ph.D. in 2009, Lowell became a Bateman Fellow at **Yale University**, where he collaborated with CDAC Partner **Kanani Lee.**

- CDAC graduate students **Matthew Armentrout (UCLA)** and **Kathryn Brown (Illinois)** were featured in the May 2012 issue of the NNSA's *Stockpile Stewardship Quarterly*.

- CDAC graduate student **Kathryn Brown**, from the research group of **Dana Dlott** at the **University of Illinois**, was awarded an Agnew National Security Postdoctoral Fellowship to carry out her postdoctoral research at **Los Alamos National Laboratory (LANL)**. **Kathryn** will be working on ultrafast spectroscopy in collaboration with **David Moore**.

- During 2011-2012, CDAC supported the participation of 6 undergraduates in **Carnegie**'s Summer Scholars Program, which is supervised by CDAC Coordinator **Stephen Gramsch**.

- Former Carnegie-CDAC Postdoctoral Fellow **Amy Lazicki** was awarded one of four Outstanding Postdoctoral Fellow Awards in the Physical and Life Sciences Directorate at **Lawrence Livermore National Laboratory (LLNL)**. Amy currently is a part of the Condensed Matter and Materials Division at **LLNL** and was a graduate student in the laser shock physics group there before coming to **Carnegie** in 2007. She returned to **LLNL** as a postdoctoral fellow in 2010.

- At **UT-Austin**, the **Lin** group collaborated with the UTeach program to provide 4th-7th grade students and teachers participating in math- and science-focused summer camps with a day-long, hands-on tour of their laboratories.

Selected Science Breakthroughs

- At **Carnegie,** a group led by **Lin Wang (HPSynC)** and including **Wenge Yang (HPSynC)**, **Zhenxian Liu (U2A)**, **Stanislav Sinogeikin (HPCAT)**, **Yue Meng (HPCAT)**, and CDAC partner **Wendy Mao (Stanford)**, along with collaborators from **Jilin University**, the **University of Nebraska**, and **Argonne National Laboratory (ANL)**, has observed a new form of very hard carbon clusters, which are unusual in their mix of crystalline and disordered motifs (Fig. 5). The material is capable of indenting diamond, which could have implications for a range of mechanical, electronic, and

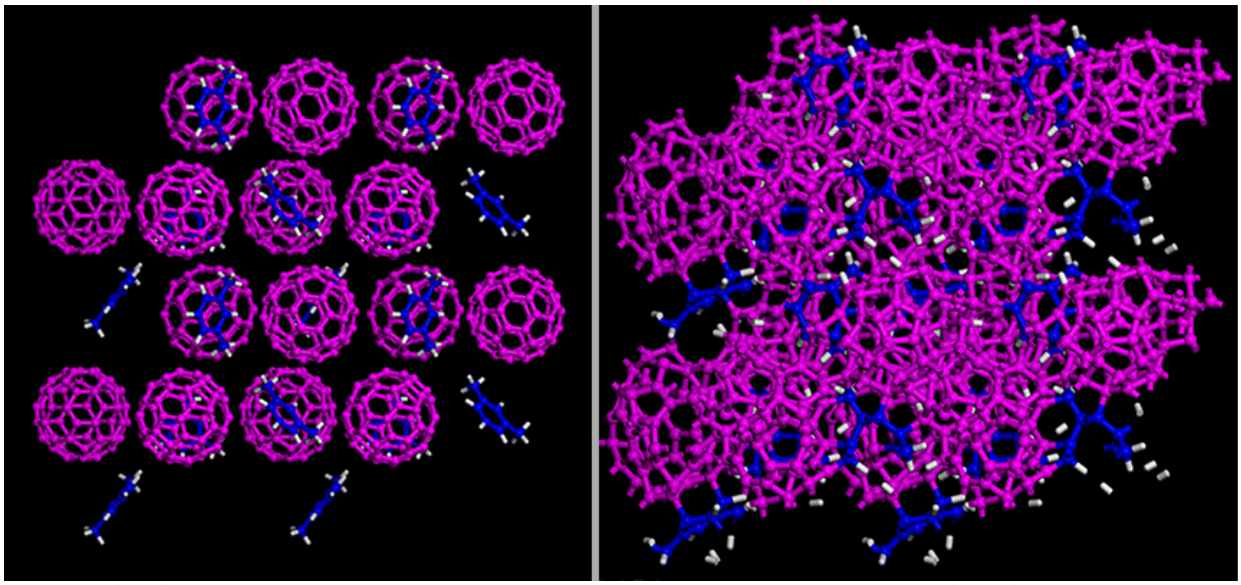


Figure 5 *(Left) C_{60} starting material showing buckyballs arranged in periodic order. (Right) under pressure buckyballs were crushed, but leaving the disordered clusters still arranged in a periodic long-range order.*[38]

electrochemical uses. Hybrid products that combine both crystalline and amorphous elements had not previously been observed, although there was some speculation that they could be created.

- Combining results from x-ray spectroscopy at **HPCAT** and neutron scattering at SNS, the **Caltech** group observed for the first time how phonons can stabilize an ordered phase more than a disordered phase. This fundamental understanding of the vibrational entropy and the interaction of

phonons and electrons at moderate temperatures could lead to more accurate predictions of stable phases in all systems. The work, led by CDAC graduate student **Jorge Muñoz**, has shown that changes in the electronic structure of a system, even when the coordination number and the bond length remain unchanged, can have important and unexpected effects on the overall thermodynamics.[3]

- **Carnegie**'s **Stewart McWilliams** and colleagues from **LLNL** and **Berkeley**, including CDAC Steering Committee Member **Rip Collins** (**LLNL**), and former CDAC Partner **Raymond Jeanloz** (**Berkeley**) studied how magnesium oxide behaves under the extreme conditions found deep within planetary interiors. Taking advantage of new laser shock compression techniques, the group found that substantial changes in chemical bonding occur as the magnesium oxide responds to dynamic compression, including transformation to a new high-pressure solid phase.[4]

- An international research team including **Wenge Yang** (**HPSynC**) and researchers from **Stanford**, **Australia National University**, **Zhizuoka University** and **Swinburne University of Technology** first synthesized the bcc phase of aluminum with an ultrafast, laser-induced, confined micro-explosion and confirmed the new phase with a high energy synchrotron x-ray micro-diffraction technique. The high pressure phase is preserved inside amorphous compressed sapphire, which is produced from a hot, dense, non-equilibrium and short-lived plasma.[5]

- The **Carnegie** team, led by CDAC Director **Russell Hemley**, developed new techniques for containing hydrogen in diamond anvil cells (DACs), allowing pressures of 360 GPa at temperatures from 12 K to room temperature. Synchrotron infrared (IR) spectroscopy was used to look for the possible dissociation of H_2 molecules and a perhaps metallic state. The intramolecular vibron persisted to the highest pressures achieved in the experiment, while the sample remained transparent in the near- to mid-IR range, indicating that the material is semiconducting, and possibly semimetallic, at these *P-T* conditions.[6]

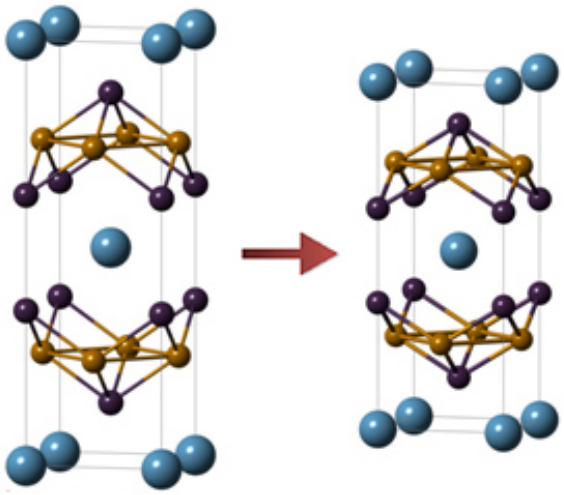


Figure 6 *The Fe-based superconductor* $(Ca_{0.67}Sr_{0.33})Fe_2As_2$ *undergoes an isostructural phase transition from a tetragonal to a collapsed tetragonal structure, in which superconductivity is observed.*

- At Carnegie, CDAC-supported Summer Scholar **Ari Benjamin** (**Williams College**) and Research Scientist **Muhtar Ahart**, along with collaborators from **LANL** applied Brillouin scattering techniques to investigating polymer behavior at high pressure, and succeeded in measuring the acoustic properties of KelF-800 to 85 GPa, much higher than achieved in previous measurements. The results of these challenging experiments show that, over the pressure range up to 85 GPa, the data on KelF-800 is best described in two separate pressure regimes, which correspond to the material before and after the collapse of the free volume.[7]

- CDAC collaborator and **Washington State University** chemistry **Choong-shik Yoo** has recently found experimental and theoretical evidence for the transformation of simple molecular carbon disulfide to an insulating black polymer with three-fold coordinated carbon atoms at 9 GPa, then to a semiconducting polymer above 30 GPa, and finally to a metallic solid above 50 GPa.[8] The metallic phase consists of a highly disordered, three-dimensional network structure with four-fold coordinated carbon atoms, in plausible structures similar to those of extended phases of its chemical analog, carbon dioxide.

- Using x-ray emission spectroscopy (XES) under pressure at **HPCAT**, **Jason Jeffries** from **LLNL** has made preliminary measurements of the Fe moment at room temperature on the iron-based

superconducting material $Ba(Fe,Co)_2As_2$. The results show a continuous suppression of the moment up to 6 GPa. and suggest that the observed superconductivity in the collapsed tetragonal phase[9] of $(Ca_{0.67}Sr_{0.33})Fe_2As_2$ (Fig. 6) exists within a lattice of magnetic Fe ions.

- At **Carnegie**, **Timothy Strobel** and CDAC-supported Summer Scholar **Viktor Rozsa** have recently discovered extremely novel behavior in hydrogen-loaded hydroquinone (ß-HQ-H_2) clathrate under pressure. Under hydrostatic compression, the volume of ß -HQ-H_2 clathrate actually expands nearly 1% when compressed between 2.5 and 3.0 GPa. Over this pressure range, the negative bulk modulus and negative linear compressibility along the *a/b*-axes are a consequence of a change in hydrogen occupancy from one to three molecules in the structure. This increase in H_2 occupancy provides insights into the design of novel molecular hydrogen storage materials with higher hydrogen capacity. The unusual negative compressibility could provide clues towards the design of novel materials with advanced properties.

- Advances in radial diffraction techniques with the DAC have allowed measurements on nanomaterials under stress and have paved the way for new types of analyses that will yield detailed information on a wide variety of samples at extreme conditions. Former CDAC graduate student **Bin Chen** (now at **Lawrence Berkeley National Laboratory**), along with CDAC Academic Partner **Hans-Rudolf Wenk** and current CDAC graduate student **Jane Kanitpanyacharoen** showed that the activities of the structural irregularities that accompany deformation occur in nickel nanocrystals 3 nm in size above 18.5 GPa. The result demonstrates that dislocation-associated deformation can take place in particles much smaller in size than computer modeling had indicated.[10]

- CDAC graduate student **Yun-Yuan Chang** (**Northwestern**) used GHz-ultrasonic interferometry to accurately quantify the elastic properties of various forms of polycrystalline diamond and related materials. These are the first measurements on polycrystalline materials made with GHz-ultrasonic interferometry and open up new territory for future ultrasonic measurements of nanoscale samples.

Technique Development

- CDAC graduate student **Kimberly Adams** (**Northwestern**) developed a sapphire-window optical cell for low-temperature synchrotron IR measurements of optical reflectance across liquid-solid transitions of light hydrocarbons at **NSLS-U2A**, in collaboration with **Bill Bassett** of **Cornell University**. Polished 1 mm culets on sapphire spheres contain the gaseous hydrocarbon and act as an IR-transparent window for the 1-5 µm spectral region of interest.

***Figure 7**. Two canted undulators installed in the Fall of 2011 at the HPCAT sector at the APS.*

- Among the many technical development projects completed recently at **HPCAT**, two undulators in canted mode were successfully installed in October 2011 (Fig. 7). In the past year, all matching optics have been commissioned, including two monochromators. The enhanced beamlines have been fully operational since November 2011. This operational mode provides two completely independent beamlines for high-pressure spectroscopy (16-ID-D) and diffraction (16-ID-B), respectively, and prepares **HPCAT** to take full advantage of the planned facility-wide APS upgrade program.

- In experiments currently being carried out at **HPCAT**, a new method of temperature measurement based on the thermoreflectance of gold is being evaluated in a collaborative effort between **Chris Seagle** and **Dan Dolan** from **Sandia National Laboratories** (**SNL**) and **Nenad**

Velisavljevic from **LANL**. The method will be used in ramp compression experiments, where temperatures are too low to measure with conventional streaked pyrometry.

2. SCIENTIFIC PROGRESS

At CDAC's beginning, the scientific program was designed as a strongly interdisciplinary effort, and this emphasis has been enhanced during the first 10 years of the Center's existence, as our Academic and Laboratory Partners have continuously pushed the frontier of high *P-T* research. As the field of high *P-T* materials science has progressed, our six original core focus areas have become more diverse, and as new research flourishes at the frontier, outstanding progress has been achieved. In our reporting, we continue to divide the scientific program into these same six focus areas, but the boundaries between these areas continue to dissolve, in keeping with true scientific advancement.

2.1 High *P-T* Phase Relations and Structures

Whether derived from experiment, theory or a combination of the two, three-dimensional structural information on materials at high *P* and *T* provides the basis for understanding how extreme conditions affect materials behavior. With the development of new tools at **HPCAT**, **NSLS**, and in the laboratories of CDAC partners, measurements at conditions that were impossible to access at the beginning of the Center are now routinely achieved. Technical improvements in experimental and computational methods are allowing CDAC groups to make demanding measurements on ever more challenging systems.

Competition and Cooperation in Silicon – Phase transformations are a fundamental aspect of high pressure research, but the atomic level details of such transformations are difficult to observe experimentally. From the point of view of thermodynamics, the free energy of one phase becomes lower than anther with pressure; the mechanism of a transformation between two solid phases, however, contains even more subtle information about how interactions between atoms of a solid evolve with increasing density. A research group from **HPCAT**, **University of Nevada-Las Vegas**, and **Jilin University** has now made careful measurements of the electron density distribution in a single crystal of silicon up to 13 GPa, the pressure of the well-known α-ß transition. As shown in Fig. 2, the electron density distribution at 12.4 GPa contains not only remnants of the low pressure structure (host lattice), but also reveals the appearance of two other groups of atoms corresponding to the atomic positions of the high pressure phase (precursor lattice). All three sets of positions are statistically occupied on the time scale of the diffraction experiment prior to the α-ß transition. First-principles calculations show that the two lattices can coexist dynamically through rapid lattice fluctuations. This interpretation provides a more detailed scheme for the phase transformation in this fundamentally important system than is possible with explanations given in the more familiar terms of displacive or reconstructive processes, and lays the groundwork for similar studies of more complex materials.[11]

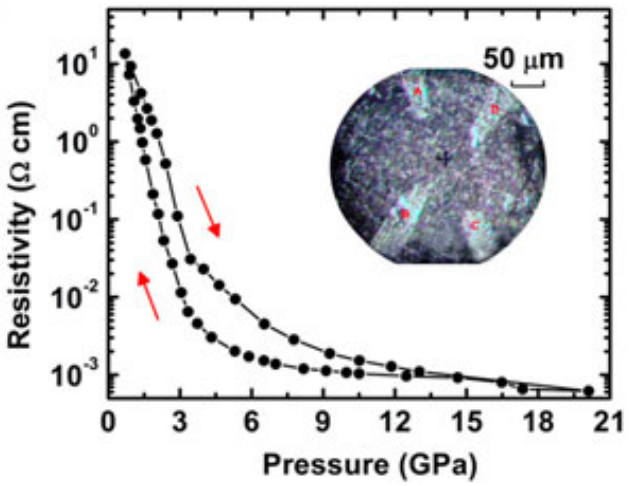


Figure 8. *Resistivity as a function of pressure for GST. Red arrows show data obtained during compression (top curve) and decompression (bottom curve). The inset shows a micrograph of the amorphous sample under pressure, along with the four electrical leads used to measure the resistance.*

High Pressure Unlocks Phase Change Mystery – **Carnegie** scientists and their collaborators have discovered new properties in the magnetic material $Ge_2Sb_2Te_5$ (GST) under pressure. Understanding and exploiting these unusual properties may eventually lead to new types of memory drives and computer

systems that store data more quickly, last longer and allow far more capacity than current data storage technologies. GST is known as a "phase change material" that, when exposed to heat, can undergo a transition between its amorphous and ordered crystalline states. The amorphous form of GST has a higher resistance to electrical current than the crystalline state, and the two phases also reflect light differently, which allows a GST-coated surface of storage media to store information and be read by miniature lasers. In addition to its improved stability compared to materials currently used in flash drives, GST has a potential response time that is 100 times faster and can be rewritten around 100,000 times.

Although GST was discovered in the early 1980s and manufactured commercially in the 1990s, the precise mechanism of the amorphous-crystalline transition has remained a mystery, partly due to unusually fast kinetics, on the order of nanoseconds, when the material is heated. To address this problem **Yue Meng** (**HPCAT**), **Wenge Yang** (**HPSynC**), and **Lin Wang** (**HPSynC**), along with colleagues from **Johns Hopkins University**, **Oak Ridge National Laboratory** (**ORNL**), **George Mason University**, and **Beijing University of Technology** used DAC high-pressure techniques to compress the material so that a gradual phase change is achieved. Using synchrotron x-ray diffraction (XRD) and electrical resistivity measurements, along with computer simulations, the group was able to isolate discrete steps in the transition between the amorphous and crystalline states and understand the process at the atomic level. The primary step in the process appears to be the reduction in volume fraction of regions of low electron density in the structure from ambient pressure to 8 GPa. This correlates directly with the drop in resistivity over several orders of magnitude observed in the same pressure regime (Fig. 8).[12]

Structural Studies on Cold Compressed Graphite – Under normal conditions, pure carbon exhibits vastly different physical properties depending on its structure. For example, graphite is soft, but diamond is one of the hardest materials known. Graphite conducts electricity, but diamond is an insulator. Graphite is the thermodynamically stable phase of carbon at ambient conditions, and the formation of diamond from graphite requires both high temperature and high pressure. The transformation from diamond back to graphite, however, is exceedingly slow.

Experimental and theoretical work has revealed other phases of carbon, indicating extensive polymorphism of both stable and metastable allotropic forms, and the potential for a variety of intriguing physical properties. Recently, at pressures of ~20 GPa, Mao et al. observed a new form of carbon formed from room-temperature compression of graphite.[13] Computational studies suggest that this material adopts a body-centered tetragonal structure characterized by four-membered rings.[14, 15]

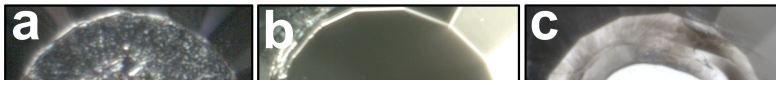


Figure 9. *Photomicrographs showing damaged diamond anvils after high-pressure experiments. (a) Photomicrograph of graphite loaded in a DAC at ambient pressure. (b) Minor scratch on the anvil surface made by M-carbon after reaching a maximum pressure of 32 GPa. The photo was taken with reflected light after the experiment. (c) Severely damaged anvil surface after reaching a maximum pressure of 50 GPa. The photo was taken with transmitted light after the experiment. The diamond culet size is 300 μm.*

Now, CDAC Partner **Kanani Lee** and postdoctoral fellow **Yuejian Wang** (Yale University) and colleague **Boris Kieffer** from **New Mexico State University** have carried out cold-compression experiments on graphite at higher pressures and provided important new information about the structure of cold-compressed graphite in this pressure regime. Known as M-carbon, this form of the element is comparable in hardness to diamond but only requires pressure to synthesize. The superhard nature of M-carbon is confirmed by its ability to damage diamond (Fig. 9). Using XRD, Raman spectroscopy, and optical techniques, experimental work has sought to verify predictions of the structure initially made in 2006. Although more than a dozen different crystal structures have

been suggested for a stable phase of carbon formed by cold compression of graphite, the proposed low-symmetry, monoclinic, M-carbon structure proposed by Li et al.[16] is the only one that fits the high pressure data[17] These findings could open the way for the synthesis of a superhard material that can withstand extreme conditions and can be used in electronic and industrial applications, as diamond-based materials are currently.

Amorphous Diamond – A High-Pressure Superhard Carbon Allotrope – The study of carbon has long been a rich and active research area offering exciting discoveries of new allotropes including both crystalline and disordered structures. Examples include such materials as buckyball, carbon nanotubes, graphene and diamond-like amorphous carbon, each having exciting potential in technological applications (Fig. 10). CDAC student **Yu Lin** and researchers from **Stanford** and **Carnegie** have observed a new carbon allotrope with a fully sp^3-bonded amorphous structure and diamond-like strength by compressing glassy carbon above 40 GPa. The initial, all sp^2-bonded glassy carbon was found to gradually transform to a fully sp^3-bonded tetrahedral carbon framework while preserving its amorphous structure. This high pressure carbon allotrope demonstrated its exceptional hardness by sustaining a pressure difference never before observed in any material besides diamond. These findings expand the wealth of pure carbon allotropes and open possibilities for potential applications using pressure-hardened, superhard amorphous solids.[18]

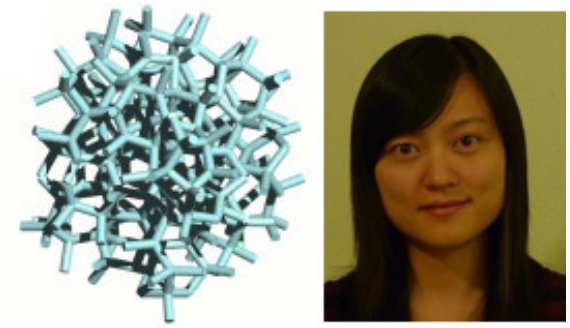


Figure 10. *Representation of an all sp^3, amorphous diamond solid. Right: CDAC graduate student* ***Yu Lin (Stanford)****.*

HPSynC Advances Nanomaterials Research – Understanding the nature of chemical bonding in carbon-based materials at high pressure is receiving increasing attention as a result of the discovery of novel structures such as carbon nanotubes and graphene. X-ray inelastic scattering spectroscopy, also known as x-ray Raman spectroscopy (XRS), has emerged as a key technique for probing the interplay between sigma- and pi-type bonding in such materials. For carbon in particular, however, the scattering from the diamonds used in the DAC tends to overwhelm the sample signal. This problem may be addressed in the XRS technique by using a radial geometry and x-ray transparent beryllium gaskets, but this requires ample space between the diamond anvils and the sample. Although the design of the DAC itself is essentially fixed, the gasket allows much more freedom for design improvements.

In recent work carried out at **HPCAT**, **Lin Wang** and co-workers from **HPSynC** have demonstrated the utility of a gasket made from a cubic boron nitride (c-BN)-epoxy composite. Used as an insert in a traditional beryllium gasket, the c-BN-epoxy composite maintains a thickness of 80 μm at 48 GPa, with 20 μm between the sample and each of the diamond anvil surfaces. With this gasket assembly, the scattering from the diamond anvils is cleanly avoided, while the scattering from the sample is maximized. This development in sampling methodology promises to significantly enhance ongoing work in the area of carbon-based nanomaterials at extreme conditions.[19]

Because the synthesis of polycrystalline samples of nanomaterials typically yields a range of particle sizes, current work is focusing on the growth and characterization of nanocrystals, with a narrow particle size distribution on the order of 100 nm. At most synchrotron facilities, however, the minimum beam size attainable is on the order of 2-5 microns, which results in a very low efficiency for diffraction measurements of nanocrystals, whereas an ideal beam size would be in the 200-600 nm range, This size of focused beam (250 nm FWHM) is provided by beamline 2-ID-D at the **APS**, and is suitable for both diffraction and x-ray imaging. Diffraction patterns taken at constant 2θ, and different azimuthal angles provides data on the compression of the nanocrystal. This work represents the first time that a nanofocused synchrotron x-ray beam has been used to study

nanoscale single crystals at high pressure, and sheds light on future studies of nanocrystals with large grain size distributions under both high pressures and ambient conditions.[20]

Element One at Extremes – Novel high *P-T* behavior in elemental hydrogen has been observed at **Carnegie** by *in situ* Raman spectroscopy. The Carnegie group studied the behavior of the symmetric stretching vibrational mode (molecular vibron) of hydrogen up to ~140 GPa and more than 1500 K and found an unexpectedly large, discontinuous softening of the vibron band over the pressure range of 30-140 GPa when the fluid phase appears at increasing temperatures (Fig. 11). Concurrently the proton bands were found to broaden and disappear. These changes indicate that the bonding is strongly altered in hot, dense fluid hydrogen.[21] Such experiments to elucidate the properties of hydrogen and its isotopes at high *P-T* conditions are important for testing predicted phase changes in the fluid phase and in the vicinity of the melting curve. Basic thermodynamic principles imply that the hot fluid is denser than the corresponding solid at pressures beyond the maximum in the melting curve. This can happen due to changes in the nature of the intermolecular and intramolecular bonding in the fluid phase. A fluid-fluid phase transition line from a non-conducting molecular phase to a disassociated conducting phase is also predicted in this *P-T* regime. Experimental efforts to verify these features have been sparse, partly because at elevated temperatures, confinement of dense hydrogen for long measurement times is challenging because of its high chemical reactivity and diffusivity.

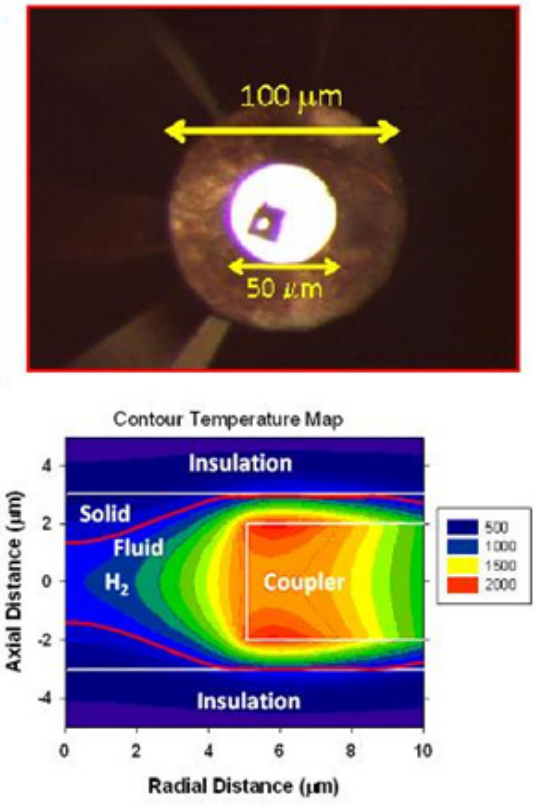


Figure 11. *Top: Typical sample assembly in which hydrogen is predominately confined in the microscopic hole drilled in an Ir coupler seen well isolated from the gasket hole (50 μm diameter region) and insulated from the anvils. Bottom: Temperature map in the sample region calculated using finite element modeling. The red line shows the fluid-solid boundary.*

The Carnegie team successfully resolved this high *P-T* confinement problem by carefully locking the hydrogen in a microscopic hole (5-8 μm diameter) drilled in an IR laser-absorbing iridium foil of thickness ~ 4 μm sandwiched in an inert buffer layer isolating two diamond anvils. To reduce the overall experiment time, a virtual experiment control and data acquisition system has also been developed for performing fully automated Raman spectroscopy measurements while samples are laser heated. These new developments have enabled studying the vibron behavior at extreme conditions over multiple heating-cooling cycles. These results are consistent with the existence of a high *P-T* transformation in the fluid related to the presence of a temperature maximum in the melting line as a function of pressure. The fluid phase formed at pressures above the melting maximum is characterized by short-range orientational order and interatomic interactions that differ from those of the fluid at lower pressures.

Polymorphism of Germanium – Like the lighter elements in its family in the Periodic Table, C and Si, the Ge crystal structure changes from the semiconducting diamond-type structure to metallic phases with increasing coordination. On the other hand, Ge has higher intrinsic electron mobilities, higher intrinsic carrier concentrations, and larger bulk excitonic Bohr radii, making it an attractive alternative to silicon for semiconductor applications. At **Carnegie**, **Xiao-Jia Chen**, **Viktor Struzhkin**, and **Ho-Kwang Mao** collaborated with **Yue Meng** from **HPCAT** on challenging

experiments designed to complete the high-pressure phase diagram of compressed Ge. Under a pressure of 66 GPa, Ge undergoes a structural change from a metallic white tin structure to an orthorhombic *Imma* structure, and then to a simple hexagonal structure at 90 GPa. These results show extraordinary agreement between theory and experiment.[22]

Superhard Tungsten Tetraboride Under Pressure – Dense transition metal borides are a new class of the growing family of superhard materials, which are extensively studied in the high pressure research community. In recent work, CDAC Partner **Abby Kavner**, CDAC student **Matt Armentrout**, and collaborators from **UCLA** examined the high pressure behavior of tungsten tetraboride (WB_4), a new candidate superhard material, up to 58 GPa. The zero-pressure bulk modulus, K_0, obtained from fitting the pressure-volume data using the second-order Birch-Murnaghan EOS is 326 ± 3 GPa. In contrast to the high pressure behavior of superhard ReB_2, an anomalous lattice softening of the *c* axis in WB_4 during compression takes place, which is partially reversible during decompression (Fig. 12). The anomaly is assigned to a second-order phase transition. It is proposed that the three-dimensional, almost isotropic, covalently bonded boron network in WB_4 is responsible for both the observed structural change in WB_4 and its high intrinsic hardness. In addition, based on the measured bulk modulus and an estimated Poisson's ratio, a high shear modulus of 249 GPa is estimated for WB_4 using an isotropic model.[23]

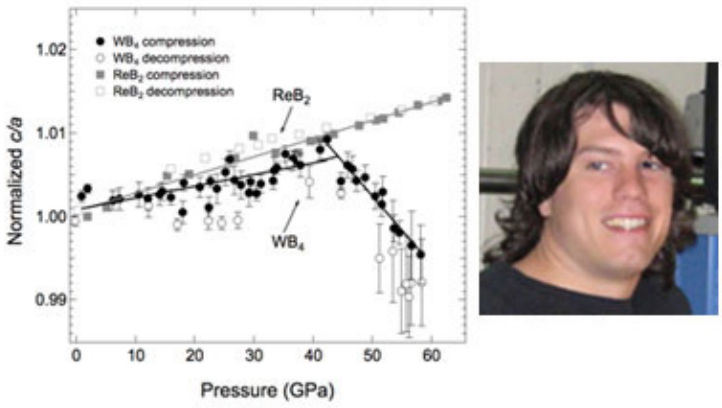


Figure 12. *Left: Variation of c/a with pressure for the WB_4 structure. The material undergoes a pressure-induced, second-order phase transition at ~42 GPa. This transition is reversible with some hysteresis, suggesting a mechanical origin. In contrast, ReB_2 shows no evidence of such a phase transition. Differences in crystal structure between the two materials can account for this observation. Right: CDAC graduate student* ***Matt Armentrout (UCLA)****.*

Post-Cotunnite Phases in the AX_2 System: Compression of PbF_2 to 80 GPa – AX_2 compounds, which include dioxides, dihalides, dihydrides and diborides, are characterized by extensive polymorphism at high pressures. The **Duffy** group at **Princeton** has been studying the sequence of phase transitions in alkaline earth difluorides, including CaF_2 and SrF_2. These materials undergo a fluorite-type to cotunnite-type phase transition and further display a cotunnite to Ni_2In-type phase transition at high pressure and temperature, with the transition pressure dependent on ionic size.[24] Lead fluoride, PbF_2, also displays a fluorite to cotunnite transition; however its transition pressure is much lower than that of the alkaline earth fluorides despite its larger ionic size, making it a good candidate for studies of post-cotunnite phases. CDAC graduate student **Camelia Stan** has investigated this sequence of phase transitions using XRD and Raman spectroscopy. Room temperature compression data yielded the previously observed isosymmetric (Pnam-Pnam) phase transition at ~14 GPa, identified as a transition from cotunnite to a Co_2Si-type structure.[25] This phase exhibits highly anomalous compressibility with the *a* axis being very compressible whereas *b* and *c* are nearly incompressible. Above 26 GPa, there is evidence for another high-pressure phase.

Single-Crystal XRD of Pyrope Garnet to 84 GPa – High-pressure XRD experiments have traditionally been based on powder diffraction. However, single-crystal diffraction has many advantages over convention powder x-ray techniques. In particular, single-crystal diffraction results in many more peaks with much better signal-to-noise ratio while avoiding ambiguities associated with peak overlap. By using small crystals in a nearly isotropic helium pressure-transmitting medium, it is possible to retain single crystals up to Mbar pressures.[26] This method provides new opportunities to obtain precise constraints on the lattice parameters, EOS, and phase transitions of

materials at high pressures. CDAC graduate student **Gregory Finkelstein** at **Princeton** is developing the use of single-crystal diffraction techniques for applications to high-pressure experiments.

The garnet structure type is of fundamental importance in Earth and materials science, but there has been minimal previous work on the 300 K compression behavior of aluminosilicate garnets at pressures higher than 10 GPa. By extending the compression of pyrope $Mg_3Al_2Si_3O_{12}$ to much higher pressures, it is possible to better constrain the EOS while also characterizing the structural response to very high pressures for the first time (Fig. 13). High pressure single-crystal XRD experiments were performed at **HPCAT** and the Advanced Light Source, and structure refinements were carried out successfully to the highest pressures, extending the range at which the compression behavior of this material has been characterized by a factor of nearly three. Pyrope exhibits smooth compression behavior and no phase transitions over the investigated pressure range. A 3rd order Birch-Murnaghan EOS was fit to the data. If the bulk modulus is fixed to 170 GPa, a value consistent with previous Brillouin scattering and ultrasonic studies, current data yields a pressure derivative of the bulk modulus of 4.8. The compression mechanisms observed for pyrope are consistent with those reported at lower pressures.

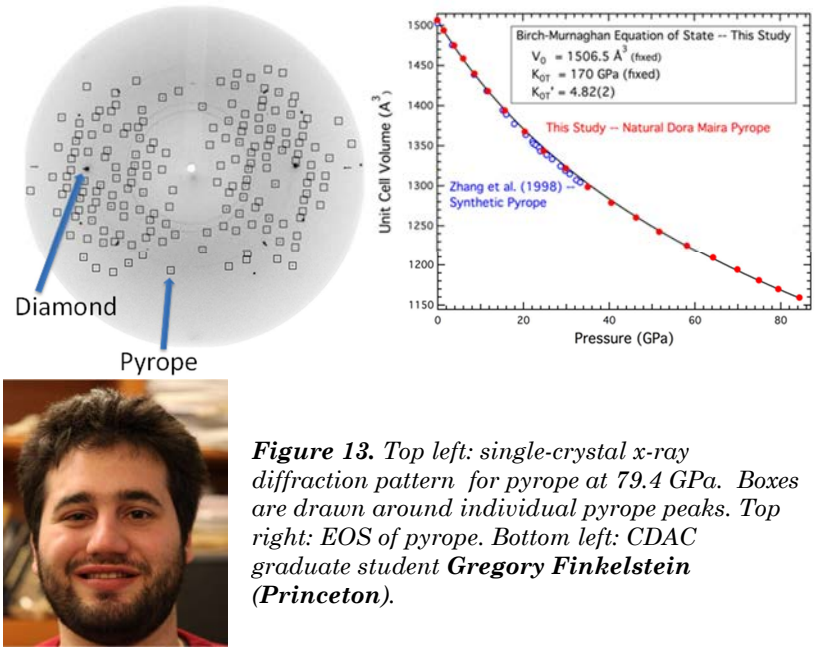


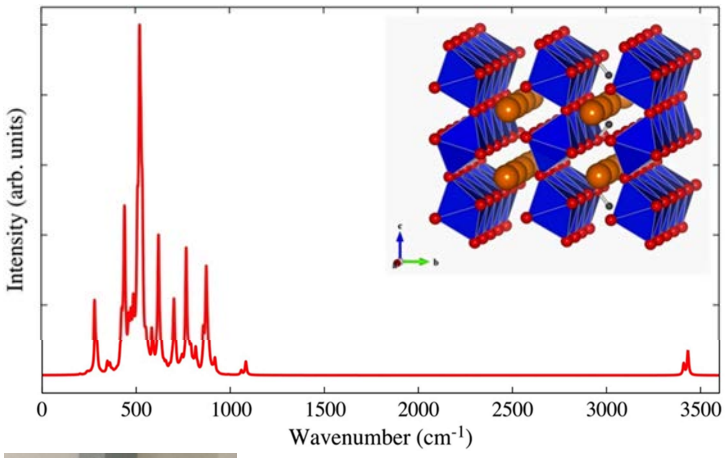
Figure 13. *Top left: single-crystal x-ray diffraction pattern for pyrope at 79.4 GPa. Boxes are drawn around individual pyrope peaks. Top right: EOS of pyrope. Bottom left: CDAC graduate student* ***Gregory Finkelstein (Princeton).***

Actinide Materials at Extreme Conditions – The **Ewing** group at **Michigan** studies the response of simple actinide oxides under extreme conditions of high pressure and energetic ion irradiation. The specific aim is to understand variations among different actinide compositions, also with respect to analog materials (*e.g.*, CeO_2). For this purpose, a large set of samples has been prepared over the last year that has been irradiated with ions and energies typical for fission fragments (185 MeV Xe). The structural behavior of UO_2, UO_3, ThO_2, and CeO_2 with accumulated radiation damage (ion fluence $1x10^{11}$ to $5x10^{13}$ ions/cm^2) have now been studied by means of synchrotron XRD measurements, along with Raman spectroscopy.

Due to their structural flexibility, pyrochlore oxides with chemical formula $A_2B_2O_7$ are important actinide-host materials. Over the last several years, the **Ewing** group has completed systematic studies on their structural response to high pressure,[27, 28] energetic ion irradiation[29, 30] and coupled effects.[31] In preparation for her research project, CDAC graduate student **Sul Gi Ye Park** has investigated the damage recovery of ion-induced amorphous pyrochlore. Two fully amorphized $Gd_2Ti_2O_7$ and $La_2Ti_2O_7$ samples were gradually annealed up to 850 °C at 1 bar, and recrystallization was monitored by means of synchrotron XRD experiments. The onset of recrystallization was at 650 °C, about 75 °C lower for the monoclinic lanthanum titanate oxide as compared with the cubic gadolinium titanate oxide. This can be understood in terms of accelerated recrystallization kinetics in forming the disordered monoclinic pyrochlore structure as compared with the highly ordered cubic phase. This result is consistent with a significantly extended temperature window for complete annealing for the latter. Within the next year, the work will continue with experiments on defect recovery and damage annealing by systematically studying the

effect of chemical composition, structure, and bond type. A main focus in this research will be also the combination of extreme conditions, such as studying the effect of high pressure on the annealing kinetics of radiation-induced amorphous samples.

Protonation of High-Pressure Silicate Perovskite Structures: Theory and Experiment – CDAC graduate student **Joshua Townsend (Northwestern)** is carrying out both theoretical and experimental studies on hydrogen incorporation into high-pressure silicates at extreme conditions, focusing on perovskite (*Pbnm*) and post-perovskite (*Cmcm*) structures (Fig. 14). To accomplish this, a collaboration has been established between the Northwestern group and **Jun Tsuchiya** at the **Geodynamics Research Center** in Japan on computational methods, and **Zhenxian Liu (Carnegie)** on the experimental approach involving synchrotron-IR at megabar pressures on laser heated samples. The perovskite structures make up the bulk of Earth's lower mantle, and developing techniques for understanding hydration of materials at extreme conditions has many applications. Hydration of post-perovskite may pertain to escape of primordial hydrogen at the core-mantle boundary. *Ab initio* calculations using density functional theory were carried out on the postperovskite form of $MgSiO_3$, which is thought to be one of the major constituents of the D" layer, just above the Earth's molten outer core. Preliminary results include several mechanically stable H defect structures. Experimental studies are underway on the laser heating of hydrated silicate starting materials at 130-150 GPa and synchrotron-IR at NSLS-U2A.



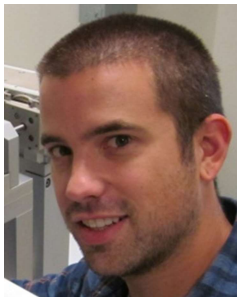


Figure 14. *Calculated IR spectrum of mechanically stable hydrous postperovskite with 0.08 wt. % H_2O. Left: CDAC graduate student* ***Joshua Townsend (Northwestern)****.*

Development of Variable Compression Rate Capability – The **LANL** group continues its work on gaining insight into the structural changes of group IV metals. The main focus has been on hafnium (Hf) and zirconium (Zr). Hf and Zr undergo a high pressure structural phase transition from a ductile α to a brittle ω phase.[32] Previous work has shown that the onset of the α → ω structural phase transition can be severely affected by such factors as experimental conditions (hydrostatic vs. non-hydrostatic) and both substitutional and interstitial impurity concentration.[33-35] Furthermore, results of previous experiments indicate that preferred crystal orientation, grain growth, transition kinetics, and other sample conditions at static high pressures can also limit the ability to detect the α → ω transition.[35] To address some of these issues, additional experiments were performed at high pressure and high compression rates in order to clarify the structural evolution, measure kinetics of structural phase transitions, and determine the reversibility of structural phase transitions in Zr and Hf.

Using a newly-developed, fast gas pressure release controller developed by the **LANL** group, **Nenad Velisavljevic** and co-workers have performed the first high pressure-variable compression rate test experiments at **HPCAT**. It has been demonstrated that a pressure increase to the membrane, on the order of 50 bar and more in less than 1s, can be achieved, resulting in a rapid pressure increase on the sample. In the first measurements it was possible to achieve pressure jumps from 1.5 GPa to 39.0 GPa in less than 2.0 s. Angle dispersive XRD patterns collected at 0.1s/spectrum using the PILATUS 100K detector reveal the structural phase transformation in Zr as

it changes from the initial low pressure hcp (α) phase into the high pressure bcc (ß) phase, as shown in Fig. 15. Previous work reported in the literature puts the ω → ß structural phase transition in Zr at ~32 GPa [32-35] and the current measurements show mostly the ß phase with some α/ω remaining at 39 GPa. These first test experiments demonstrate the feasibility of achieving high pressures at high compression rates with a DAC and further experiments are planned in order to determine the α/ω/ß phase ratio as a function of compression (*i.e.*, strain) rate. Following the initial jump to 39 GPa, pressure remains very stable within ± 0.5 GPa over the next 30s, which is crucial in carrying out further experiments to determine kinetics of structural phase transitions.

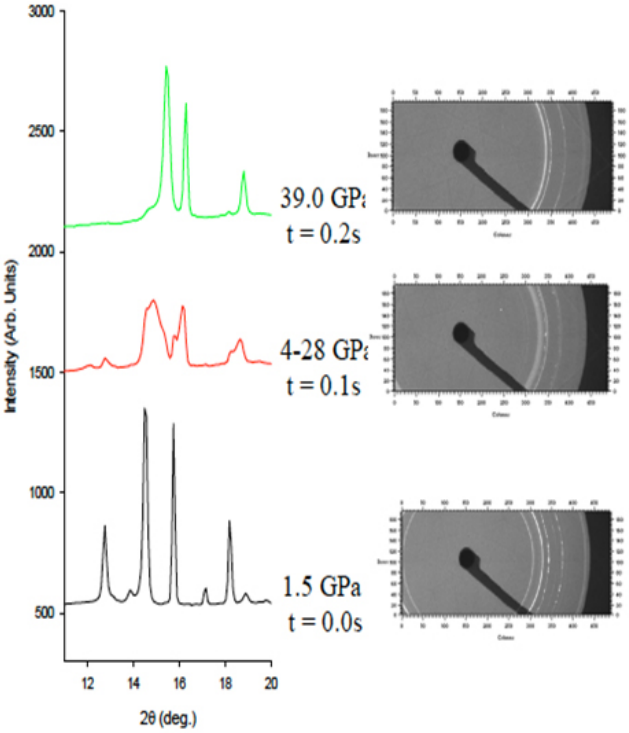


Figure 15. *ADXD Spectra collected during a high compression rate experiment on Zr. During a pressure jump (in 0.2s or less) Zr undergoes a structural phase transformation from the low-pressure α phase at 1.5 GPa to the high-pressure ß phase with some α/ω remaining at 39 GPa.*

Distinct Superconducting States in the Nominal Semimetal Bi_4Te_3 – The compound Bi_4Te_3 is a member of the infinitely adaptive $(Bi_2)_m(Bi_2Te_3)_n$ series.[36] This series is composed of alternating and interwoven layers of Bi_2 and Bi_2Te_3 quintuple layers. The $(Bi_2)_m(Bi_2Te_3)_n$ series includes elemental Bi, which is a semimetal, and the topological insulator and thermoelectric material Bi_2Te_3 as end members. At ambient pressure, Bi_4Te_3 is a semimetal, but, under pressure a series of structural transitions reconstructs the electronic structure yielding metallic behavior, as evidenced by the dramatic change in the Hall coefficient under pressure.[37] In work carried out at **HPCAT**, **Jason Jeffries (LLNL)** has been investigating the structural behavior of these materials at high pressure. The transitions proceed similarly to those of elemental Bi, first to a monoclinic phase, and ultimately to a body-centered-cubic (bcc) phase at the highest pressures. This bcc phase is an alloy, with Bi and Te occupying the sites of the bcc cell with stoichiometric, but presumably random, occupancy. Similar to the end members of the infinitely adaptive series, Bi_4Te_3 exhibits superconductivity in the metallic structures. The superconducting critical temperature, T_c, in the monoclinic phase increases with pressure from approximately 2 to 4 K. The phase transition at 14 GPa to the *bcc* alloy elevates T_c to about 8 K. Further pressure suppresses T_c, as is expected for a phonon-mediated superconductor. The phase transition sequences, the occurrence of a pressure-induced *bcc* alloy, and the development of superconductivity in the $(Bi_2)_m(Bi_2Te_3)_n$ series suggests universal high-pressure behavior. Understanding how the disparate ambient-pressure states of the series converge to this universal high-pressure behavior could provide insights into the conditions that favor topologically protected surface states.

Titanium Dioxide Nanotubes at High Pressures – Titanium dioxide (TiO_2) nanotubes have shown remarkable properties in a variety of applications, such as gas sensors, photoelectrochemical generators, solar cells, and as a drug delivery platform. It is well established that bulk TiO_2 undergoes a phase transition sequence from either the anatase or rutile phase to the α-PbO_2 phase, and then to the baddeleyite-type phase under high pressure. However, nanostructured materials often exhibit dramatically different behaviors than the corresponding bulk materials. CDAC collaborator **Yang Song** from the **University of Western Ontario** systematically studies the high-pressure behavior of TiO_2 nanotubes in terms of phase transitions, phase stability, and

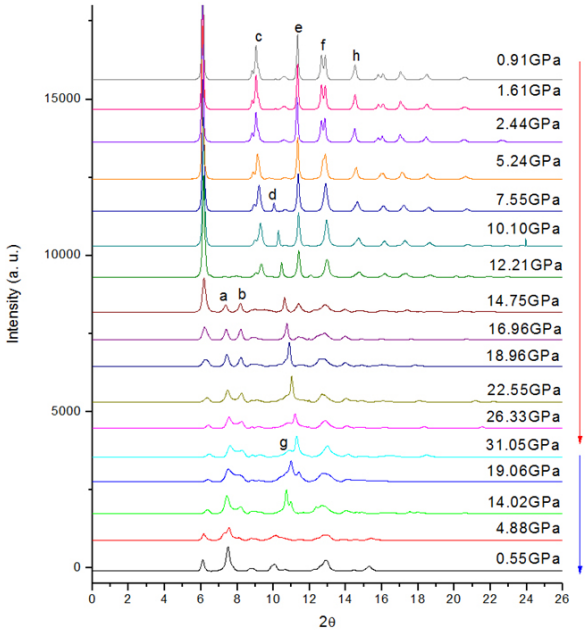


Figure 16. *X-ray diffraction patterns for TiO_2 nanotubes. The red and blue arrows indicate the compression and decompression sequence, respectively.*

compressibility to gain an in-depth understanding of the pressure-morphology effect on TiO_2 nanomaterials by using *in situ* x-ray micro-diffraction at **HPCAT**. XRD measurements were performed on TiO_2 nanotubes upon compression up to 31 GPa (Fig. 16). The diffraction pattern measured at 0.9 GPa can be indexed on the anatase structure with good quality. When the pressure reaches 7.6 GPa, a reflection *d* at 2θ=10° appears and the double peaks at 2θ ~12.7° merges into a single reflection. With increasing pressure, the intensity of reflection *d* increases, but the intensity of the reflections *c, e* and *h* at 2θ=9°, 11.3° and 14.5° which represent the anatase phase, decrease and disappear at 19.0 GPa. Meanwhile, two reflections *a* and *b* at 2θ=7.3° and 8.2° appear when pressure reaches 12.2 GPa. This indicates that a new phase of TiO_2 is formed at 7.6 GPa as anatase begins to convert into a new phase. When the pressure reaches 19.0 GPa, anatase is completely converted to the new phase. Upon decompression to near ambient pressure, the corresponding back transformation is not observed, indicating the pressure-induced phase transitions are irreversible.

Order in Disordered Carbon – At **Carnegie,** a group led by **Lin Wang (HPSynC)** and including **Wenge Yang (HPSynC)**, **Zhenxian Liu (U2A)**, **Stanislav Sinogeikin (HPCAT)**, **Yue Meng (HPCAT)**, and CDAC partner **Wendy Mao (Stanford)**, along with collaborators from **Jilin University**, the **University of Nebraska**, and **Argonne National Laboratory (ANL)**, has observed a new form of very hard carbon clusters, which are unusual in their mix of crystalline and disordered motifs. The material is capable of indenting diamond, which could have implications for a range of mechanical, electronic, and electrochemical uses. Hybrid products that combine both crystalline and amorphous elements had not previously been observed, although there is some speculation that they could be created.

The synthesis starts with C_{60} cages; xylene solvent was then diffused into the spaces between the cages to form a new structure. Pressure was then applied to this combination of carbon cages and solvent, to see how it changed under different stresses. At relatively low pressure, the cage structure remained, but as the pressure increased, the cage structures started to collapse into more amorphous carbon clusters. However, the amorphous clusters still occupy their original sites, forming a lattice structure. There appears to be a narrow window of pressure, around 32 GPa, in which this material is created and does not revert to the cage structure when pressure is removed. This material is capable of indenting the diamond anvils, as illustrated in Fig. 17. If the solvent used to prepare the new form of carbon is removed by heat treatment, the material loses its lattice periodicity, indicating that the solvent is crucial for maintaining the chemical transition that underlies the new structure. Because there are many similar solvents, it is theoretically possible that an array of similar, but slightly different, carbon lattices could be created using this pressure method.[38]

Successive Structural Transitions in Relaxor $Pb(In_{1/2}Nb_{1/2})O_3$ – Pb-based perovskite relaxor ferroelectrics and related materials are currently used in a new generation of electromechanical devices, owing to their high piezoelectric coefficients with electromechanical deformations one order of magnitude larger than those of conventional $PbZrO_3$-$PbTiO_3$ (PZT) ceramics. While extensive theoretical and experimental studies have advanced our understanding of relaxors, their properties are still poorly understood.

At **Carnegie**, **Muhtar Ahart** investigates the $Pb(B'_{1/2}B''_{1/2})O_3$-type relaxors, in which the degree of cation ordering at the B-site can depend on the nature of heat treatment at high temperatures. $Pb(In_{1/2}Nb_{1/2})O_3$ (PIN) has different chemical orderings in the arrangement of In^{3+} and Nb^{5+} on the B-site depending on different thermal treatment and can be classified into three groups, which are called (a) ordered PIN, disordered PIN, and (c) partially disordered PIN. It has been reported that ordered PIN shows a first-order phase transition from the paraelectric phase (*Fm*-3*m*, Z=8) to the antiferroelectric phase (*Pbam*, Z=8) at about 160 ºC. The disordered PIN shows relaxor behavior characterized by a dielectric dispersion below 50 ºC, and partly disordered PIN shows a broad peak in the dielectric constant without dielectric dispersion about 90 ºC. Raman scattering and XRD have been used to investigate the behavior of PIN under pressure up to 50 GPa at 300 K. A sharp peak near 370 cm^{-1} in the Raman spectra increases in intensity with pressure (Fig. 18). The linewidth of the band at 550 cm^{-1} also increases with pressure, and two of the Raman peaks merge above 10 GPa. The structural phase transition is particularly associated with the splitting of the 50 cm^{-1} peak above 16 GPa. In most Pb-based relaxors other than PIN, the Raman band at 50 cm^{-1} shows a slight hardening with pressure, but no splitting is observed at higher pressure. The pressure evolution of the diffraction patterns for PIN shows obvious splitting above 16 GPa, particularly for pseudo-cubic (110), (111) and (220) diffraction peaks; this indicates a symmetry-lowering transition in PIN. PIN therefore appears to undergo successive structural phase transitions. The transition at 6 GPa is similar to the one observed in other Pb-based relaxors and is related to octahedral tilting. The transition at 16 GPa could be a rhombohedral to orthorhombic transition, and the transition at 38 GPa could be an orthorhombic to monoclinic transition. Ongoing work will seek to resolve these outstanding structural issues.

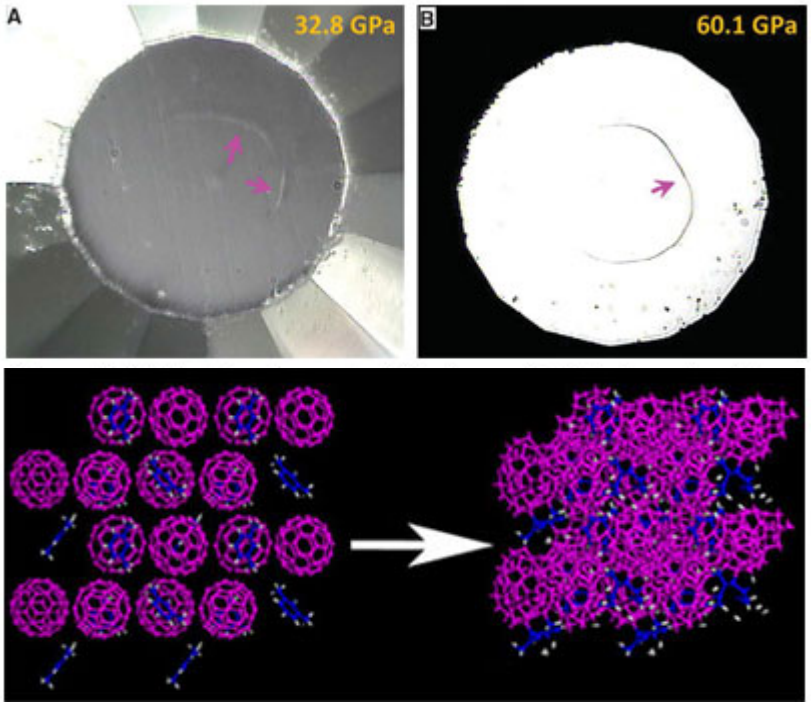


Figure 17. *Top: Optical photomicrographs of the ring cracks in the diamond anvils generated after formation of a crystalline-amoprphous hybrid material and then release of pressure. The maximum pressures were 32.8 (A) and 60.1 (B) GPa. As marked by the arrows, the ring cracks follow the original boundary of the samples in the gaskets. Bottom: Carbon clusters in a model of the crystal structure before and after compression.*

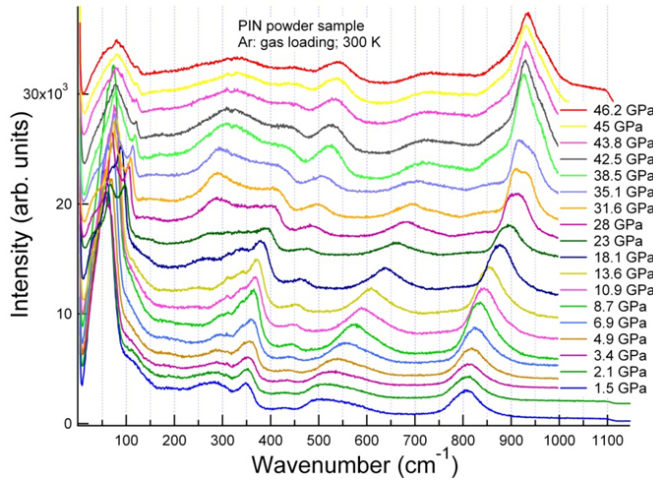


Figure 18. *Raman spectra with pressure for $Pb(In_{1/2}Nb_{1/2})O_3$ at 300 K.*

2.2 *P-V-T* EOS Measurements

Over the past 10 years, we have seen an increasing emphasis on the development of dynamic compression methods for understanding materials at extreme conditions. This in turn demands ever higher resolution in static measurements, with the ultimate goal of merging static and dynamic methods for understanding materials at conditions relevant for stockpile stewardship. A wide variety of materials are studied by CDAC personnel, from metals and crystalline compounds to polymers and other amorphous solids, and even to liquids and other types of fluids.

Internally Consistent Pressure Scale to 2.5 Mbar – Accurate pressure measurements are essential for experimental studies of phase transitions and physical properties of materials under extreme pressure conditions. Pressure scales based upon shock compression experiments suffer from uncertainties at high compression due to corrections for thermal effects. Independently derived pressure scales from shock data have been observed to deviate increasingly with pressure to as much as 10% at Mbar pressures.[39] The **Duffy** group at **Princeton** has conducted synchrotron XRD experiments in the DAC in which combinations of Au, MgO, Mo, NaCl (B2) and Pt, Ne, and He are compressed together. From this data set, it has been possible to derive internally consistent pressure scales for these materials under quasi-hydrostatic conditions to 250 GPa for the first time. The resulting EOS parameters for Au, Pt, and Mo are all in excellent agreement with independent shock compression data. Deviatoric stresses at 2.5 Mbar are similar for experiments conducted in Ne and He media. The new comprehensive pressure scale reduces pressure differences among this group of calibrants from 10% to 3% in the 1.5-2.5 Mbar range (Fig. 19). Improved pressure calibration at multi-megabar pressures will benefit many types of experiments conducted at these extreme pressure conditions. This work formed part of the PhD thesis of CDAC graduate student **Susannah Dorfman**.

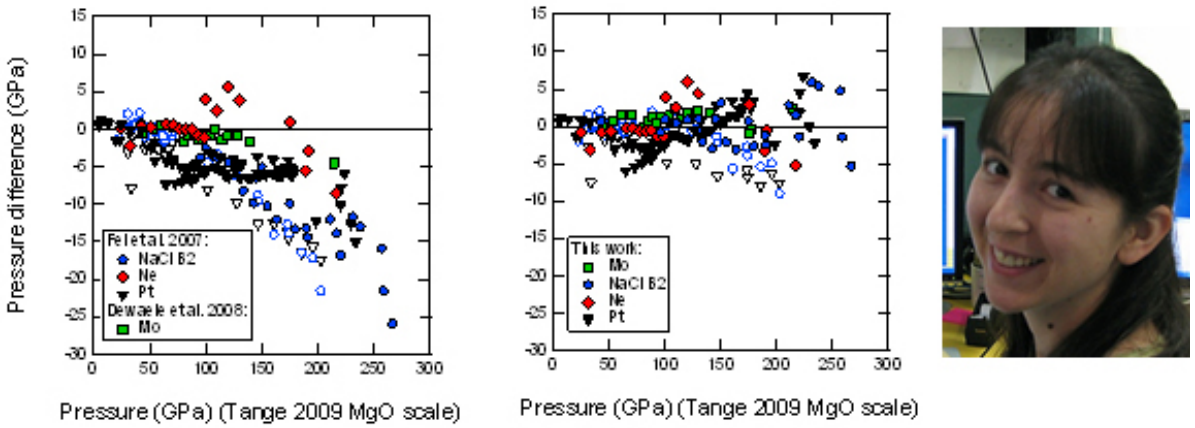


Figure 19. *Differences between pressures determined from unit cell volumes of Au, MgO, Mo, NaCl (B2), and Pt simultaneously observed in this work (filled symbols) and previous studies (open symbols).[40-43] The reference is the MgO equation of state of Tange et al.[44] Left panel shows pressure differences using previous equations of state of Fei et al.[45] and Dewaele et al.[39] The right panel shows the improved agreement resulting from the simultaneous fit to the combined data set.*

Nonhydrostatic Compression of Ruby from Radial XRD up to 68 GPa – The strength and mechanical properties of hard ceramic materials are required for applications under extreme static and dynamic mechanical stresses and high pressures.[46] Ruby (α-Al_2O_3: Cr^{3+}) is important as a widely-used pressure standard for static high-pressure experiments in DACs.[47] The properties of Al_2O_3 have also recently been investigated extensively under dynamic compression.[48, 49] However, the strength and mechanical properties of ruby under static loading are not well characterized.[50] CDAC graduate student **Susannah Dorfman** at **Princeton** has measured the lattice strain and stress state of polycrystalline ruby up to 68 GPa under non-hydrostatic compression using angle dispersive XRD in a radial geometry. The measured differential stress increases with pressure, and ruby can support a

stress of 16 GPa at a mean pressure of 68 GPa (Fig. 20). The observed strength of ruby increases from 3.4 % of the shear modulus at 19 GPa to 6.3% of the shear modulus at the highest pressure. The increase in strength is similar to that observed in shock compression experiments at much higher strain rates,[49] but is different from that previously reported in diamond cell experiments.[50] Comparing the data for ruby to high-pressure data on a wide range of other hard ceramics, the results show that the high-pressure yield strength correlates better with hardness than with either the bulk or shear modulus.

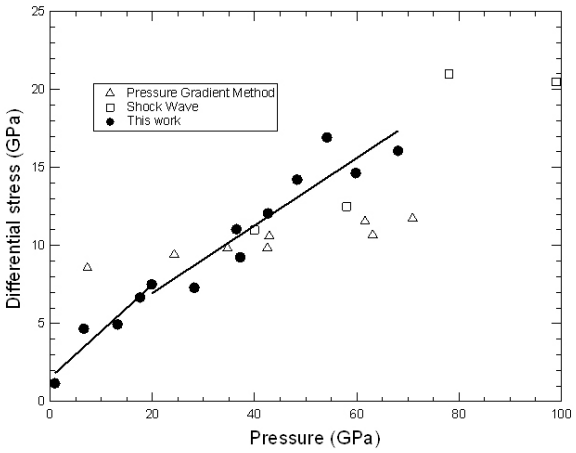
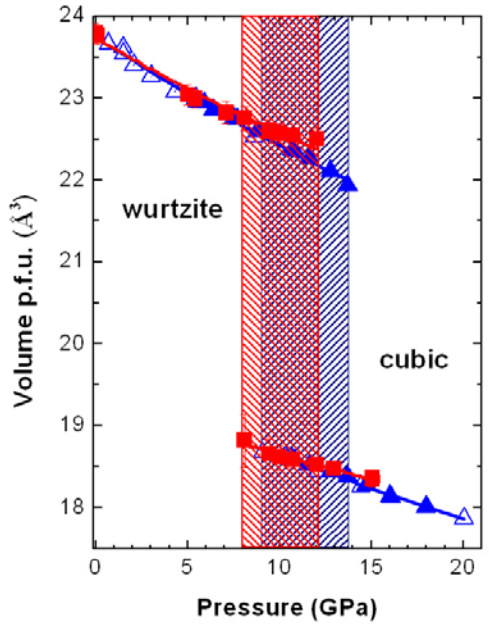


Figure 20. *Differential stress in ruby (Cr-doped Al_2O_3) from radial x-ray diffraction measurements. A peak differential stress of 16 GPa at 68 GPa mean pressure was found in these experiments. Also shown in the figure are previous diamond anvil cell experiments based on the pressure gradient method and strength measurements under shock compression.*

Stability and EOS of $BaCO_3$ to 150 GPa and 2000 K – The structures of XCO_3 carbonates (X = Ba, Pb, Sr, Ca, Mg) under high *P-T* conditions do not appear to follow systematic trends with increasing ionic radius of the X cation. Whereas the aragonite (*Pmcn*) to post-aragonite (*Pmmn*) transition pressure of $BaCO_3$ (~8 GPa), $PbCO_3$ (~17 GPa), $SrCO_3$ (~35 GPa) and $CaCO_3$ (~40 GPa) increases with their metal ionic radii, the post-postaragonite structure ($C222_1$) predicted for $CaCO_3$ and $MgCO_3$ has not been observed experimentally in $BaCO_3$. In order to test for further phase transformations and to measure the compressibility of post-aragonite $BaCO_3$, CDAC graduate student **Joshua Townsend** from the **Jacobsen** group **Northwestern** conducted synchrotron XRD and *in situ* laser heating experiments on $BaCO_3$ to 130 GPa and 2000 K at **HPCAT**. $BaCO_3$ has the aragonite structure at ambient conditions. On heating to 1100 K at 5.5 GPa, $BaCO_3$ adopts the *Pmmn* post-aragonite structure, in agreement with previous experimental studies. After heating the sample to 1800-2000 K at various pressures between 10 and 150 GPa, all diffraction patterns can be assigned to the orthorhombic *Pmmn* structure, although the a and c axes merge and become similar within uncertainty above 70 GPa. In agreement with *ab initio* and molecular dynamics studies, a transformation to a pyroxene-like $C222_1$ structure predicted for $MgCO_3$ and $CaCO_3$ is not observed. The wide stability field of the orthorhombic *Pmmn* structure of $BaCO_3$ to 150 GPa and 2000 K is remarkable, and is accompanied by a dramatically higher bulk modulus than previously thought, with K_0 = 115(7) GPa, compared with previous estimates of K_0 = 84 GPa.



Fiugre 21. *Pressure dependence of the volume per formula unit for bulk and nanocrystalline ZnO. Triangles (blue on line) – bulk ZnO sample. Squares (red on line) - ZnO nanopowder. Open symbol: data taken with silicon oil as a pressure transmitting medium (PTM), solid symbols: with neon as a PTM. Shaded areas are the pressure ranges for which both phases coexist. Lines represent fits to the Murnaghan EOS.*

Optical and Mechanical Properties of Nanomaterials – An ongoing theme in the **Saxena** group at **Florida International** has been the application of high pressure experiments to study zinc oxide phases, which

have gained substantial interest in recent years. ZnO is an attractive material for future developments in optoelectronic, spintronic, and sensor applications. Established values of bulk moduli for both the wurtzite and sphalerite phases are quite scattered. One of the possible reasons for such a large scattering of the values of bulk moduli could be associated with the quality of the sample material. Work on this project was focused toward a comparison of the elastic properties under high hydrostatic pressure of very high quality bulk ZnO crystals with those of ZnO nanocrystals using synchrotron XRD and optical photoluminescence. It was found that compressibility of ZnO is indeed considerably smaller for ZnO nanocrystals. Results also show that the transition from the wurtzite to the sphalerite phase occurs at slightly lower pressures for nanocrystalline ZnO than for bulk crystals, and that the ranges in which both phases coexist are different for bulk and nanocrystalline samples (Fig. 21). Contrary to theoretical expectations, no additional intermediate phase of ZnO is detected, either for bulk or for nanocrystalline samples.

P-T Phase Diagram of Ammonium Nitrate – Previous work by **Raja Chellappa** at **LANL** established the *P-T* phase diagram (Fig. 22) of ammonium nitrate [AN: NH_4NO_3] using synchrotron XRD experiments conducted at **HPCAT**.[51] This is the first revision of the AN phase diagram in over 50 years for this extremely important compound, which is widely used in explosive formulations. Phase boundaries representing transitions to the high temperature polymorphs and liquid were determined during multiple *P-T* measurements using both diffraction and Raman spectroscopy measurements. Polymorphism in AN is well known to be very complex, with at least five structurally distinguishable phases whose *P-T* stability can depend on variety of factors including humidity, transformation kinetics and sample history. High resolution diffraction measurements at **HPCAT** were required to carefully identify phase transition *P-T* conditions. At room temperature, the ambient pressure orthorhombic (*Pmmn*) AN-IV phase was stable up to 45 GPa with no evidence for phase transitions. AN-IV was also observed to be stable in a large *P-T* phase space. The phase boundaries are steep with a small phase stability regime for high temperature phases. A *P-V-T* EOS based on a high temperature Birch-Murnaghan formalism was obtained by simultaneously fitting the *P-V* isotherms at 298, 325, 446, and 467 K, thermal expansion data at 1 bar, and volumes from *P-T* ramping experiments. Anomalous thermal expansion behavior in AN was observed at high pressure with a modest negative thermal expansion in the 3-11 GPa range for temperatures up to 467 K. The role of vibrational anharmonicity (particularly the modes associated with NO_3^- moieties) in this anomalous thermal expansion behavior has been established using high *P-T* Raman spectroscopy. It has been demonstrated that the intrinsic anharmonicity (pure temperature effect of volume expansion) increases with pressure. Additional high *T* measurements are needed in the low pressure regime (0–5 GPa) to improve the accuracy of the proposed phase boundaries as well as to further investigate the anomalous thermal expansion behavior of AN-IV.

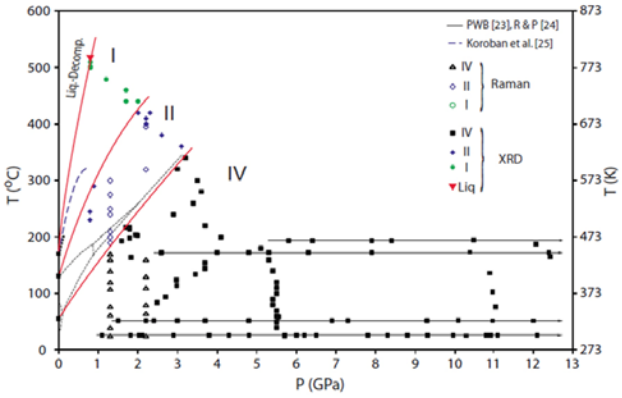


Figure 22. *Revised P-T phase diagram of AN (solid red lines) based on XRD and Raman measurements. The solid-solid phase boundaries from earlier studies are shown as black dotted lines and the melt/decomposition line shown as a dotted blue line. The phase stability of AN-IV extends up to 40 GPa at 298 K and 37 GPa at 467 K.*

Helium Stiffens Glass under Pressure – SiO_2 glass is a prototypical network-forming glass with a high degree of intermediate range order. The open structure of SiO_2 glass makes it highly compressible, with molar volumes decreasing sharply with pressure exceeding those of crystalline polymorphs of quartz and coesite at around 20 GPa and approaching that of dense stishovite at 40 GPa. When SiO_2 glass is loaded with helium under pressure, however, it becomes much less compressible. The stiffness may be a result of helium entering in the voids in SiO_2 glass under

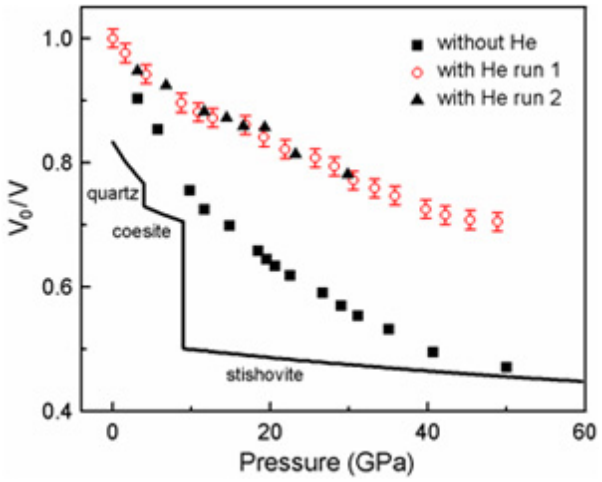


Figure 23. *Pressure dependence of the molar volume of SiO_2 glass with helium loading in this work and without helium from literature data. The thick black line represents the EOSs of crystalline polymorphs of SiO_2.*

pressure. Incorporation of helium in SiO_2 glass is verified by XRD and Raman spectroscopy. Data measured at **HPCAT** show that the position of the first sharp diffraction peak (FSDP) for SiO_2 glass in a helium medium remains essentially the same under pressures up to 18.6 GPa, which is in stark contrast to that of SiO_2 glass without a pressure medium, where the large increase in density under pressure has been attributed to significant modification of the intermediate range ordered structure manifested by a drastic change in the FSDP in the structure factor. The observed preservation of the FSDP may reflect an effect of dissolved He on the structure of SiO_2 glass and, therefore, the compression mechanism (Fig. 23).

Experiments on GeO_2 glass and SiO_2 glass with H_2 as a pressure medium do not show this stiffness effect, implying that size plays a major role in understanding the effect. Any elements or molecules with kinetic diameters larger than that of H_2 (0.29 nm) apparently cannot enter the voids of the glass in a sufficiently large amount. So far, the effect of helium on the structure and compression of SiO_2 glass is found to be unique, because of the combination of controlling factors including the small kinetic diameter of helium, the high degree of intermediate range order in SiO_2 glass, and the large fraction of interstitial solubility sites occupied by helium.[52]

2.3 Phonons, Vibrational Thermodynamics, and Elasticity

In addition to accurate structural information and reliable EOS parameters, vibrational properties of materials provide critically needed thermodynamic information for understanding and predicting materials behavior at extreme conditions. CDAC scientists use synchrotron XRD, x-ray spectroscopy and IR spectroscopy along with Brillouin spectroscopy to address a variety of key physical properties and their evolution with pressure and temperature.

Thermal Conductivity of Materials at High Pressure – Measurement of the thermal properties of materials at high pressure represents an important advance in high pressure research, and has been an ongoing theme in the CDAC scientific program for the past several years. In the group of CDAC Partner **David Cahill** at **Illinois**, graduate student **Wen-Pin Hsieh** extended the experimental technique of time-domain thermoreflectance (TDTR) to the high-pressure environment of diamond and SiC anvil cells and applied these methods to fundamental studies of the thermal conductivity of materials and the thermal conductance of interfaces.

Disordered Materials – The model of the minimum thermal conductivity[53] reliably predicts the thermal conductivity of most simple amorphous solids. Recent computational work, however, has suggested that localized modes and anharmonic interactions might play a significant role in determining thermal conductivity of glassy polymers.[54] **David Cahill**'s group at **Illinois** has measured the thermal conductivity of poly (methyl-methacrylate) (PMMA) brushes grafted from SiC anvils to $P \approx 10$ GPa.[55] The pressure dependence of the thermal conductivity is in good agreement with the trends predicted by the model of the minimum thermal conductivity calculated using data for the pressure dependence of the elastic constants of PMMA measured by picosecond acoustics. In the high pressure limit, $P > K$, where K is the bulk modulus. Simple theory predicts that the thermal conductivity of amorphous materials and strongly disordered crystals will scale approximately with $P^{1/2}$. Data for PMMA are in agreement with this expectation, as shown in Fig. 24, despite the fact that the simple theory does not take into account the complexity of the molecular structure of a glassy polymer.

Pure Crystals – For crystalline materials, the Leibfried-Schlömann (LS) equation is often used to predict the pressure dependence of the thermal conductivity, but the LS equation has never been tested over a wide range of compression. In a collaboration with CDAC Partner **Jie Li** (**Michigan**) and graduate students **Bin Chen**, **Wen-Pin Hsieh** and **David Cahill** used TDTR and DAC techniques to measure the thermal conductivity[56] of water ice phase VII to 22 GPa. At this pressure, the molecular volume of H_2O has been reduced to 63% of the volume at 2 GPa and the thermal conductivity increases by nearly an order of magnitude, in good agreement with the behavior predicted by the LS equation. The agreement between theory and experiment suggests that heat transport by optical phonons is negligible in comparison to heat conduction by acoustic phonons. The L-S equation predicts that the thermal conductivity of a pure crystal will scale approximately with $P^{3/2}$ in the limit of high pressure.

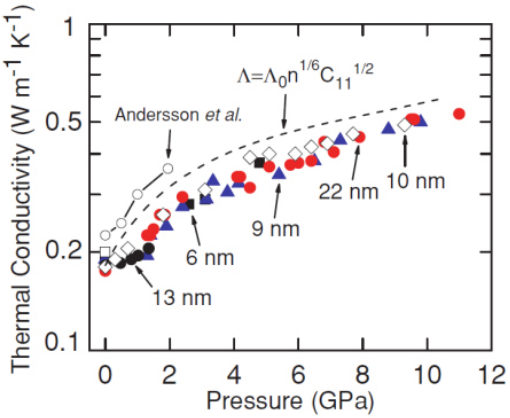


Figure 24*. Measurements of the thermal conductivity of PMMA brushes (solid symbols) and a spun-cast layer (open diamond) as a function of pressure. The dashed line shows the predicted thermal conductivity based on the minimum thermal conductivity model. Data for bulk PMMA (open circles) are included for comparison.*

In collaboration with **Alexander Goncharov** and **Allen Dalton** at **Carnegie**, **Hsieh** and **Cahill** have extended TDTR to pressures as high as 60 GPa. MgO has emerged as a testbed for both theory[57, 58] and experiment[59-61] on the thermal conductivity of materials under extreme conditions. **Hsieh** and **Dalton** solved problems with polishing and sample preparation and completed measurements to 60 GPa at room temperature using Al transducers. The thermal conductivity is in good agreement with the prediction of theory, as shown when the Grüneisen parameter γ is calculated from the MgO equation-of-state reported by Zha et al.[62]

Thermal Conductance of Weak Interfaces – The acoustic mismatch model (AMM) and diffuse mismatch model (DMM) are often used to predict and interpret the thermal conductance G of an interface between two materials. These models assume that G is a consequence of only the lattice dynamics of the bulk materials on each side of the interface; changes in the bonding and vibrational density of states of atoms adjacent to the interface are not explicitly accounted for in these models.

High-pressure environments enable continuous tuning of the lattice dynamics of materials through the anharmonicity of atomic or molecular bonds. For interfaces, anvil cell techniques can easily generate the high pressures, typically $P \approx 10$ GPa, needed to increase the small force constants characteristic of van der Waals interactions to values more typical of strong chemical or ionic bonds. Figure 25 shows that, as the strength of interface bonding increases at high pressures, the thermal conductance of weakly-bonded interfaces approaches the thermal conductance of clean and strongly-bonded interfaces between materials. This is the first systematic experiment on the effects of interfacial bonding on thermal transport.

Cahill and graduate student **Greg Hohensee** are now focusing on the opposite limit of this same science, *i.e.*, the situation where the experimental values for G are much larger than can be accounted for by simple models.[63, 64] A larger than expected G is often observed when the materials on the two sides of the interface have highly dissimilar lattice vibrations, *e.g.*, Pb/diamond. The highest frequency phonon in Pb is only ≈ 2.2 THz; at phonon frequencies < 2 THz, the phonon density of states in diamond is extremely small compared to Pb. G for Pb/diamond interfaces is typically observed to be an order of magnitude larger than the so-called "radiation limit" for harmonic phonon transport.

One possible explanation for the observed high values of G is that phonons in diamond can couple not only with one-phonon states of the material on the other side of the interface but also with two-phonon states created by anharmonicity. **Hohensee** and **Cahill** are testing this idea by

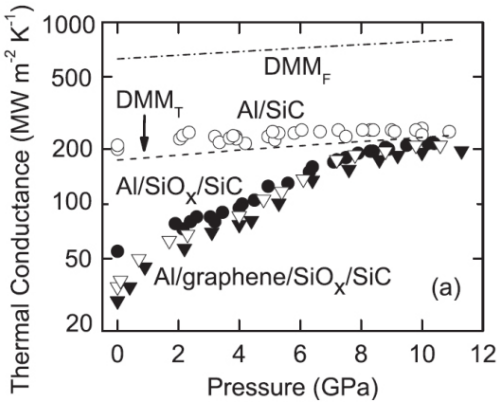


Figure 25. *Pressure dependence of the thermal conductance G(P) of various Al/SiC interfaces. G(P) of the clean Al/SiC interface (open circles) is weakly dependent on pressure. By contrast, G(P) of the weak interfaces Al/SiOx/SiC (solid circles) and Al/graphene/SiOx/SiC (open and solid triangles) increases rapidly with pressure due to the increasing interface stiffness and approaches the value of the clean Al/SiC interface at P > 8 GPa. The DMM prediction for G(P) of the Al/SiC interface is shown as the dashed line for two limiting cases of the phonon densities of states.*

measuring *G* for interfaces between highly dissimilar materials at pressures up to 50 GPa. In initial experiments (Fig. 26), a dilute alloy of Pd in Au is deposited directly on the face of the diamond anvil.[65] High pressure is needed to significantly alter the phonon density of states of Au.

At ambient conditions, we observe a value for *G* that is comparable to the two-phonon radiation limit and appears to scale, at least initially, as predicted by the changes in the phonon spectrum of Au with pressure. These data support the idea that phonon thermal transport at these interfaces is governed by the coupling of one-phonon states in diamond to two-phonon states in Au. Currently work is focused on extending these studies to the more extreme case of Pb/diamond.

Rare Earth Impurities in bcc Fe: Structure, Dynamics, and Pressure Effects – In the **Fultz** group at **Caltech**, **Lisa Mauger** and **Sally Tracy** have begun an effort toward understanding 4f-3d electron bonding by mixing rare earth elements with iron. The solubility of rare earth elements in bcc Fe is notoriously low, and Fe does not dissolve well into hcp rare earth metals. **Mauger** and **Tracy** have found that it is possible to mix Dy and Fe by thermal evaporation onto a cold substrate. The result is an amorphous alloy. The concentration of the alloy is challenging to control, but chemical analysis has shown that the compositions of the alloys are Fe-50at%Dy and Fe-75at%Dy. General user beamtime was obtained to perform nuclear resonant inelastic x-ray scattering (NRIXS) of ^{57}Fe on these Fe-Dy alloys under pressure at Sectors 3 and 16 of the APS, to measure how the phonon partial DOS of Fe is changed as the interactions of 3d and 4f electrons are altered. The thin films were loaded into panoramic DACs and gave phonon spectra at 27 and 29 GPa, as shown in Fig. 27. The phonon partial DOS curves of the amorphous alloys of alloys of Fe-50at%Dy and Fe-75at%Dy were not significantly different at ambient pressure, but they seem reasonably consistent with the Fe phonon

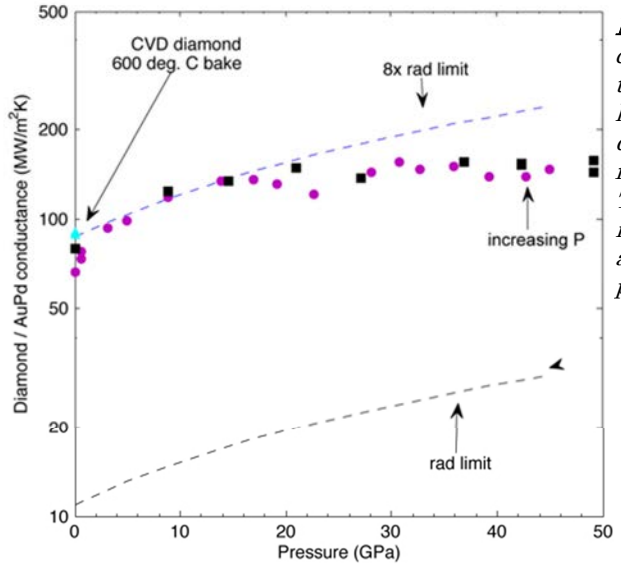
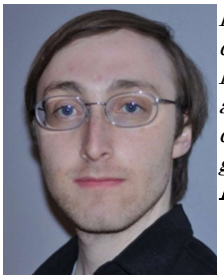


Figure 26. *Far left: Measurements of the thermal conductance G of a Au(Pd) alloy film deposited on the face of a diamond anvil. The x-axis is the hydrostatic pressure within the volume of the diamond anvil cell as measured by ruby fluorescence. The y-axis is the thermal conductance. The filled circles labeled "increasing P" are measured while loading the cell; the filled squares are measured while reducing the pressure. The one-phonon radiation limit is shown as the lower dashed line. For the two-phonon density of states, the radiation limit is larger by a factor of 8, and is shown by the upper dashed line. Left: CDAC graduate student* ***Greg Hohensee*** *(**Illinois**).*



partial DOS curves of Fe-Tb reported by Ruckert, et al.[66] The two curves were also similar under pressure. This indicates that in an amorphous structure, there is not a large chemical difference in the quasiharmonic phonon stiffening, even though the numbers of Fe-Dy pairs should be much larger in the Fe-50at%Dy alloy than in Fe-75%Dy.

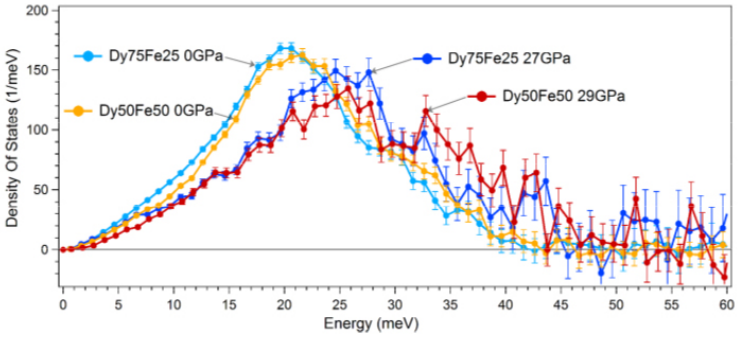


Figure 27. Phonon partial DOS of ^{57}Fe measured by NRIXS on amorphous thin films of Fe-Dy alloys.

Unexpected Effect of Atomic Vibrations on the Phase Stability of FeV – The Fultz group at **Caltech**, along with colleagues from **ORNL**, the **Air Force Research Laboratory**, and **Carnegie** have observed for the first time how vibrations of atoms in a crystal lattice (phonons) can stabilize an ordered phase more than a disordered phase. This is the reverse of what has been exclusively observed until now; usually the stronger chemical bonds of an ordered phase cause its atoms to vibrate less at a given temperature, giving it the lower vibrational entropy. The work was carried out by CDAC graduate student **Jorge Munoz** (**Caltech**), along with CDAC graduate student **Lisa Mauger** and former CDAC students **Matt Lucas** and **Mike Winterrose** (all from **Caltech**), and **HPCAT** beamline scientists **Paul Chow** and **Yuming Xiao**.

The higher vibrational entropy of the ordered phase in the equiatomic alloy FeV, which has a body-centered cubic parent lattice, determined by combining measurements from inelastic neutron scattering (INS) performed at the ARCS instrument at the Spallation Neutron Source (**ORNL**) and nuclear resonant inelastic x-ray scattering (NRIXS) performed at **HPCAT**. This allowed for an accurate determination of the phonon density of states (DOS) and the study of iron and vanadium motions separately through their partial DOS (pDOS) curves, as shown in Fig. 28. It was observed that all the vibrations shift to lower energies and have higher entropy upon ordering, but the effect is more prominent for low-energy transverse vibrations than for longitudinal vibrations. The effect is also stronger for vanadium atoms than for iron atoms. The origin of this phenomenon was shown by computational work to be at the level of the electrons. The ordered alloy has more electrons available to screen the displacements of moving atoms, especially the vanadium atoms. This new correlation between the change in the electronic structure of a particular atom in a system and the shift in energy of the pDOS of that atom may be more general and can be used to study other systems. A fundamental understanding of the vibrational entropy and the interaction of phonons and electrons at moderate temperatures could lead to more accurate predictions of stable phases in all systems. This work has shown that changes in the electronic structure of a system, even when the coordination number and the bond length remain unchanged, can have important and unexpected effects on the phonon DOS and the overall thermodynamics.[3]

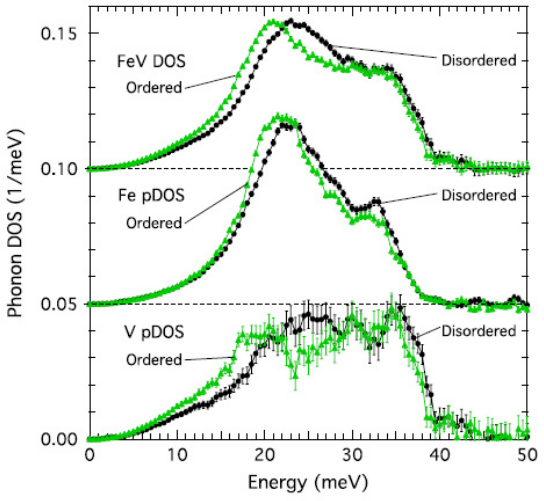


Figure 28. Neutron weight corrected phonon DOS curves of FeV samples (top panel), along with Fe pDOS curves (middle panel), and V pDOS curves (bottom panel). The Fe pDOS curves were determined directly by NRIXS measurements; the total FeV DOS curves and the V pDOS curves by inelastic neutron scattering.

Elastic Moduli of Nanopolycrystalline Diamond – CDAC graduate student **Yun-Yuan Chang** (Northwestern) is using GHz ultrasonic interferometry to accurately quantify the elastic properties of various forms of diamond and related

materials. Knowledge of the elastic properties of superhard materials is important to characterizing their novel properties relative to diamond. This year, in collaboration with **Tetsuo Irifune** (**Geodynamics Research Center,** Japan), **Chang** measured ultrasonic sound velocities in a 6-mm rod of GRC nanopolycrystalline diamond (NPD).

Using ultrasonic-pulse overlap methods from 0.7-1.4 GHz, the sound velocities of GRC-NPD were measured with high accuracy (Fig. 29). This is the first polycrystalline material measured with GHz ultrasonic interferometry and opens up new territory for future ultrasonic measurements of nanopolycrystalline materials. Because acoustic wavelengths in materials at GHz-frequencies are typically on the order of a few micrometers, most polycrystalline materials do not transmit the GHz ultrasound. In a 6 mm rod of the NPD, good transmission of over a thousand acoustic wavelengths, corresponding to three round trips through the sample, or a travel distance of nearly 40 mm, was observed. Therefore, grain boundaries of GRC-NPD do not scatter acoustic waves at near-optical wavelengths. No shear-wave anisotropy was observed, consistent with a uniform distribution of crystallite orientations. The resulting bulk modulus $K = 442.3$ (±1.0) GPa, shear modulus $G = 532.3$ (±0.6) GPa, and Young's modulus $E = 1140$ (±2) GPa are comparable to natural diamond.

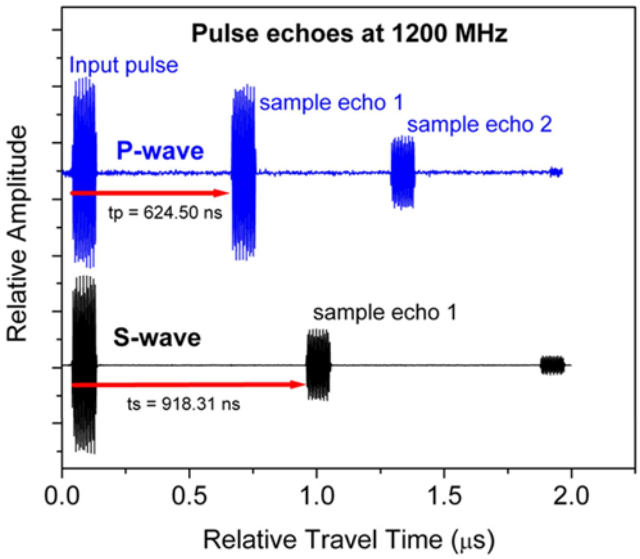


Figure 29. *GHz-ultrasonic pulse echoes in a 6-mm rod of nanopolycrystalline diamond. Acoustic-wave travel times were used to determine the elastic moduli of NPD with an uncertainty of less than 0.2%. Right: CDAC graduate student* ***Yun Yuan Chang*** *(**Northwestern**).*

Thermoelastic Properties of ReB_2 at High Pressures – The **Kavner** group at **UCLA** has extended the pressure and temperature conditions of the measured structural stability and thermoelastic properties of ultrahard ReB_2. This data is important for understanding the basic physics of this class of materials and for guiding the design of new materials. As part of this effort, CDAC graduate student **Matt Armentrout** has measured the phase stability and thermoelastic EOS of ReB_2 at pressures up to 30 GPa and temperatures up to 2500 K using a laser heated DAC at **HPCAT**. ReB_2 is shown to be stable throughout this pressure and temperature range. ReB_2 has a small thermal anisotropy, but a large mechanical anisotropy. Combining this new data set with previously existing results from a large volume press yields a thermoelastic EOS with a Grüneisen parameter of 2.40 (0.08) and a q of 2.7. A comparison of ReB_2 with high electron density, incompressible elemental metals shows that ReB_2 has the lowest thermal pressure at moderate compressions and a low thermal expansivity combined with high bulk modulus through a broad range of pressures.

Sound Velocities in Earth's Inner Core – Earth's inner core exists at over 360 GPa pressure and temperatures perhaps in the 6000 K range. While remote, its existence affects the geodynamo and how the Earth's interior has evolved through time. A number of enigmatic properties of the Earth's inner core have been recently discovered, including variable seismic speeds and differential super-rotation in which the inner core is observed to be rotating at a different speed from the rest of the planet. Deciphering these observations requires a knowledge of the composition of the Earth's inner core and the sound velocities and densities of candidate iron alloys at high pressures and temperatures.

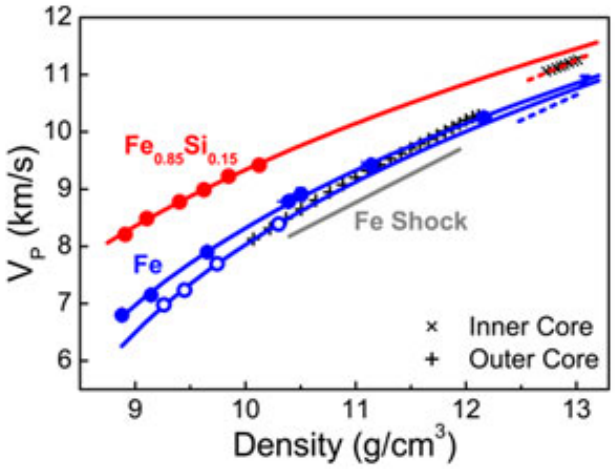


Figure 30. *Compressional wave velocity and density profiles of iron and iron-silicon alloy at high pressures and temperatures. The dashed lines show the velocity and density relations of iron (blue line) and iron-silicon alloy (red line) at 6000 K.*

alloys to constrain the chemical composition of the Earth's core using seismic observations. Indications are that Earth's inner core, with approximately 8 wt% silicon can have a velocity-density profile at 6000 K that matches well with seismic observations of the region (Fig. 30).[67]

Thermal Conductivity at Extreme Conditions – The conduction of heat in materials at extreme conditions is important in many processes, including the dynamics of deep planetary interiors, fast chemical reactions and explosions. With pulsed laser heating, extreme temperatures are also accessible in addition to the pressures provided by DACs. Under these conditions, however, it is difficult to measure how materials conduct heat. To better understand the thermal conductivity of materials at very high pressures, **Carnegie** CDAC-affiliated scientists **Alexander Goncharov**, **Allen Dalton**, **Viktor Struzhkin**, and **J. G. O. Ojwang**, along with former Carnegie Summer Scholar **Michael Wong** (**Berkeley**) and colleagues from **Uppsala Unviersity** have measured the thermal conductivity of solid Ar using a novel method. A thin film of iridium metal was placed in a DAC and surrounded with argon gas. The pressure was increased to 50 GPa, where the Ar gas became a solid layer around the iridium foil. Brief laser pulses were then used to heat

This area of research is pursued extensively in the group of **Jung-Fu Lin** at **UT-Austin**. Led by CDAC student **Jeff Liu**, and former CDAC student **Zhu Mao** (**Princeton**, now a postdoctoral associate at **UT-Austin**), the group recently measured the compressional wave velocity and density of iron and iron-silicon alloy at pressures over a megabar and at high temperatures to understand the physical and chemical properties of Earth's core. The experiments were carried out using advanced inelastic x-ray scattering and XRD techniques. Results from these measurements show that high temperature significantly decreases the compressional wave velocity of iron in the hexagonal close packed structure at high pressures, and the iron-silicon alloy exhibits similar high-pressure behavior to pure iron with a constant density offset. Together with previously published results, the group has created a new velocity-density model of iron

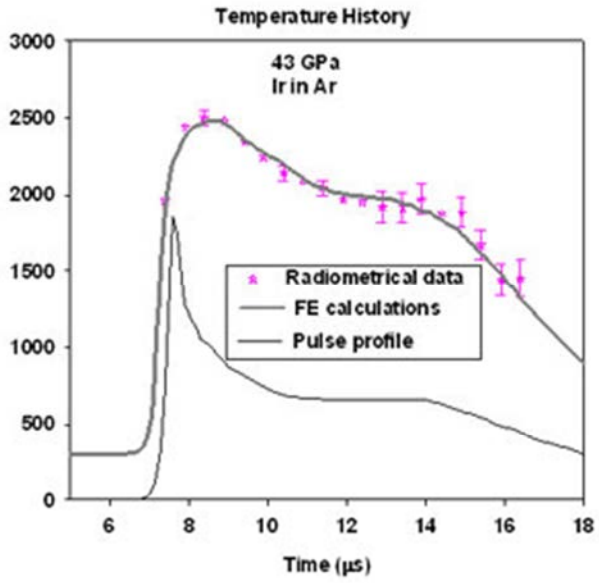
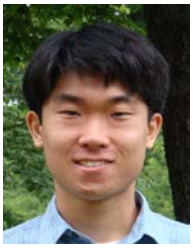


Figure 31. *Time-resolved spectroradiometry results from a sample of solid Ar at 43 GPa. Close agreement is obtained between experimental observations and finite element (FE) calculations of the temperature of the samples as a function of time. The spectra are used to calculate the thermal conductivity of Ar. Right: CDAC Summer Scholar* ***Michael Wong (Berkeley)****.*



the sample to 2,500K. The microsecond laser pulses produced a temporal thermal profile across the solid argon sample (Figure 31).

By measuring the temperature history of the iridium foil, it is possible to calculate the thermal conductivity of the surrounding argon medium. The thermal conductivity of argon at high pressure can be explained using a straightforward model based on kinetic theory, as illustrated by the close fit of the data points with finite element calculations. These results and new methodology are crucial for ongoing studies of how minerals behave in the Earth's mantle. The results are also important to the broader high pressure research community because argon is used as a pressure transmitting medium in many DAC experiments. A more complete understanding of the behavior of argon at high pressures therefore will result in more accurate measurements of the properties of materials in extreme environments.[68]

2.4 Plasticity, Yield Strength, and Deformation

Understanding the behavior of key materials at high plastic strain and high strain rates is crucial for stockpile stewardship. Texture data provides a means for interpreting active deformation mechanisms, and phase transformations induced by pressure and temperature produce systematic changes in texture patterns. Studies of these and related phenomena at ultrahigh pressures have become routine as a result of the development work carried out in a number of CDAC research groups at **HPCAT** and HIPPO.[69] Technical advances at both facilities promise to continue supporting this fundamental area of research well into the future.

Crystallographic Preferred Orientation in FeO – Magnesiowüstite (Mg,Fe)O, also known as ferropericlase, is one of the key minerals that make up the Earth's lower mantle. The stoichiometric endmember FeO does not exist in nature, but compositions close to the 1:1 elemental ratio are common. FeO is a fundamentally important material in its own right, not only for its geophysical relevance, but also as a member of the transition metal monoxides, which serve as important examples for comparison between condensed matter theory and experiment. For this reason, the high pressure behavior of FeO has been the subject of intensive study for nearly 50 years.

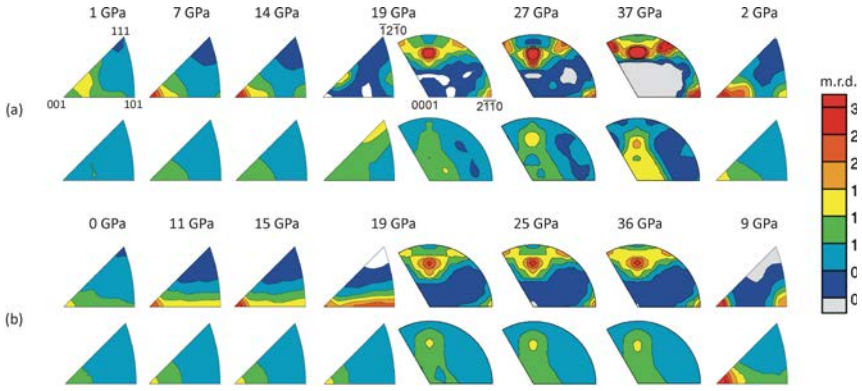


Figure 32. *(a) Inverse Pole Figures showing textural evolution of ($Mg_{0.08}Fe_{0.92}$)O up to 36.6 GPa through the phase transition from cubic to rhombohedral and returning to cubic upon decompression; compression direction shown in top row, and axis perpendicular to the compression direction shown in second row. (b) Texture evolution of $Fe_{0.94}O$ up to 36.2 GPa. Texture sharpness is measured in multiples of the random distribution (m.r.d.). Equal area projections.*

In a recent investigation, CDAC graduate students **Pamela Kaercher**, and **Jane Kanitpanyacharoen**, along with CDAC Partner **Hans-Rudolf Wenk** (**Berkeley**), former CDAC Student **Lowell Miyagi** (**University of Utah**), and colleagues from the **Geoforschungszentrum** in Potsdam, Germany, compressed two powdered samples, ($Mg_{0.08}Fe_{0.92}$)O magnesiowüstite and $Fe_{0.94}O$ wüstite, non-hydrostatically up to ~37 GPa at ambient temperature in the DAC in order to observe textural evolution as a function of pressure.[70] Under uniaxial stress {100}c planes aligned perpendicular to the compression direction for both ($Mg_{0.08}Fe_{0.88}$)O and $Fe_{0.94}O$ (Fig. 32), and texture sharpness increased with pressure. Near 19 GPa and room temperature, cubic FeO transitioned to rhombohedral symmetry. Polycrystal plasticity simulations show that deformation in the cubic phase of the (Mg,Fe)O solid solution to be due mostly to slip on {110}<1-10>c as previously found for other

B1 structures. In the rhombohedral phase, slip system activity changed slightly with one of the daughters of ({111}<1-10>c, {10-11}<-12-10>r, inactive in the cubic phase), becoming active.

Texture near the transition pressure suggests that crystals in the cubic phase with their {100}c planes facing the compression direction are preferentially oriented to transform to the rhombohedral phase first. Orientations that developed and strengthened in the rhombohedral phase remained after decompression back to the cubic phase. Upon decompression, a texture similar to that of the cubic phase before the phase transition was observed, suggesting a perfect memory during this displacive transition.

Fiber Reinforced Composites under Pressure – Understanding the relationship between applied macroscopic stress and microscopic lattice strain of controlled-geometry multiphase composites in the DAC is a key interest of the **Kavner** group at **UCLA**. In a recent study, a composite material consisting of oriented Al_2O_3 fibers embedded in an Al metal matrix was sliced in two different orientations, and thin sections were prepared. Samples were then loaded into the DAC in two different orientations, an NaCl pressure calibrant was included, and XRD was measured as a function of temperature and pressure at **HPCAT**.

Preliminary results from this study show that, as expected, the lattice strain behavior is indeed sensitive to the orientation of the composite within the diamond cell compression axis and the lattice strains of Al and Al_2O_3 behave differently. An unexpected result is that the behavior of the lattice strain of Al relative to Al_2O_3 falls outside of the bounds of constant stress/constant strain relationships, as shown in Fig. 33. These results raise troublesome questions about measurements of equations of state in the DAC using an internal pressure calibrant and also raise fascinating questions about the macroscopic and microscopic stress/strain relationships of mechanical mixtures under extreme conditions. Elucidating some of these questions and addressing them in a quantitative manner is a goal of **UCLA**'s future work in the CDAC program.

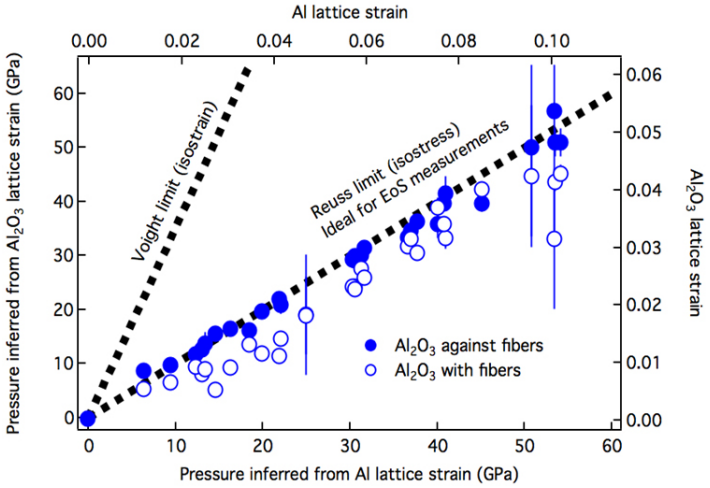


Figure 33. *Plot of the pressure inferred by referencing the measured Al_2O_3 lattice parameters to its equation of state as a function of the pressure inferred by the measured Al lattice parameter. The black dashed line of slope 1 represents the Reuss (stress continuity) bound. The Voigt (constant strain) bound is plotted as a second black dashed line. The filled symbols show the Al_2O_3 lattice strain from composites oriented in the diamond cell perpendicular to the fiber orientation. In this direction there is stress continuity. The open symbols show pressures from the lattice strains measured parallel to the fiber axis. These fall outside the limits of the Voigt-Reuss boundary.*

High-Pressure, High-Temperature Microstructure Evolution of Metals – The development and healing of crystal defects, which have first-order control on the creep mechanism in the deformation and material transport in high-pressure, high-temperature metals, is a focus of the **Panero** group at **Ohio State**. Initial experimental samples, prepared by CDAC graduate students **Jeff Pigott** and **Dan Reaman**, are composed of a 10 µm thick, $Fe_{64}Ni_{36}$ alloy foil, cleaned of oxidation under high vacuum (10^{-10} torr) with an electron beam. Without exposing the sample to air, a uniform layer (300-500 nm) of Ni or Fe is sputtered onto the surface of the substrate. The samples are loaded into a DAC with Ar as the pressure medium. After compression and laser heating, foils are extracted from the diamond cell for *ex situ* analysis. Using FIB milling, a ~100-200 nm thick slice is extracted through the center of the heated spot, removed and thinned to electron transparency.

The microstructure of these samples with respect to dislocation densities has been analyzed with respect to variations in pressure and temperature. Initial results show that the effect of 50 GPa

hydrostatic pressure noticeably increases the defect density. The defects in these alloys appear very similar to the defects that occur in shocked steels (Fig. 34, left),[71] with the development of twins upon α - ε phase transitions. It has been observed that locations of twinning occur in regions of a high defect density in the foil as rolled, leading to regions of shear localization in the room temperature samples, which can explain the observations of non-homogeneous distribution of defects upon shock loading. Laser heating to 95% of the melting temperature, however, significantly anneals defects on timescales of < 1 minute (Fig. 34, right). Significant mixing is observed between the pure deposited layer and the alloy substrate, indicating transport times 2-5 orders of magnitude in excess of those expected by lattice diffusion. These results indicate that material transport is occurring along grain boundaries and through defects.

Metal foils used in most high-pressure, high-temperature experiments are rolled at moderate to low temperatures. This causes a significant grain preferred orientation and a high density of defects. The defect density then affects the reactivity and the solid-state deformation at high pressures and temperatures. Understanding of annealing of defects at high pressures becomes crucial for the interpretation of the nanoscale compositional measurements.

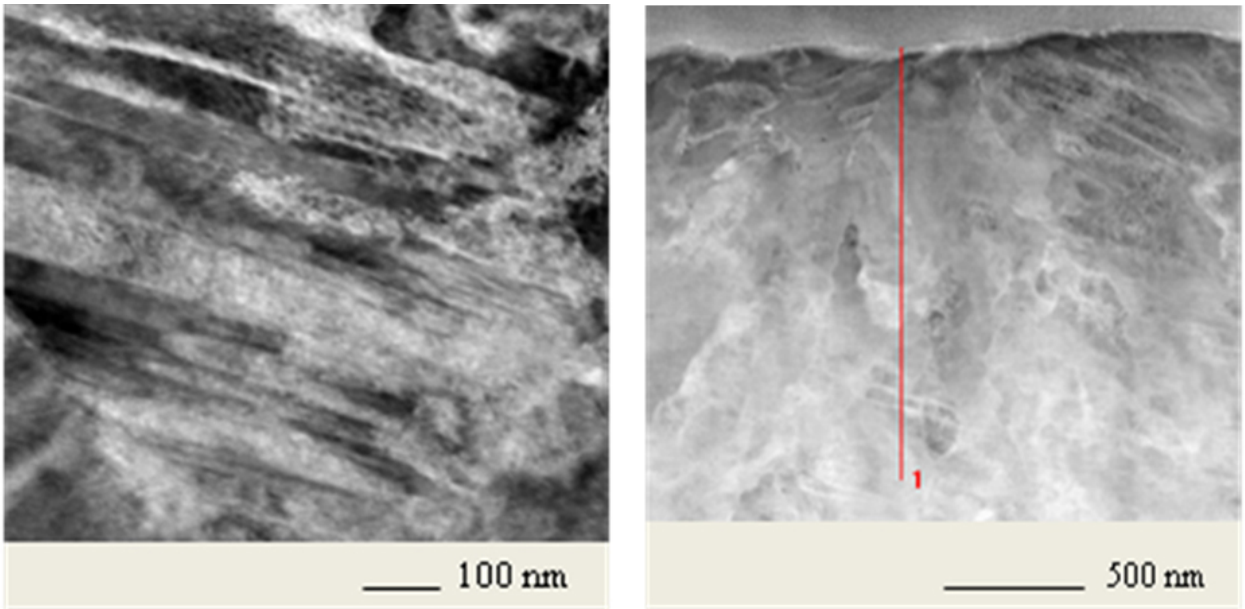


Figure 34. *TEM micrographs of iron-nickel alloys hydrostatically compressed to 60 GPa (left) at room temperature and (right) heated to ~2900 K for 50 s showing a significant healing of defects through heating. Note the different length scales.*

Building Better Structural Materials – When a material is subject to external stresses, it will eventually change its shape. Initially, such changes are elastic and reverse when the stress is relieved. When the intrinsic strength of the material is exceeded, however, the changes become permanent and can result in breaking or shattering, but permanent changes in shape are also possible. Understanding the behavior of nickel nanocrystals at high pressure is the focus of current research by former CDAC student **Bin Chen** (now at **Lawrence Berkeley National Laboratory**), CDAC Partner **Hans-Rudolf Wenk** (**Berkeley**), CDAC Student **Jane Kanitpanyacharoen** (**Berkeley**), and colleagues from **LBNL**, **Berkeley**, **UC–Santa Cruz**, and **Southern University**. Recent findings could help physicists and engineers create stronger, longer-lasting materials, and also help earth scientists understand tectonic events and seismicity (Fig. 35). It is believed that permanent changes taking place in metallic grains under pressure are associated with the movement of dislocations. However, the deformation of nanocrystalline materials has been controversial because it was thought that below a certain grain size, these structural irregularities would not form and the deformation would instead be dictated by motions of the boundaries between grains. According to

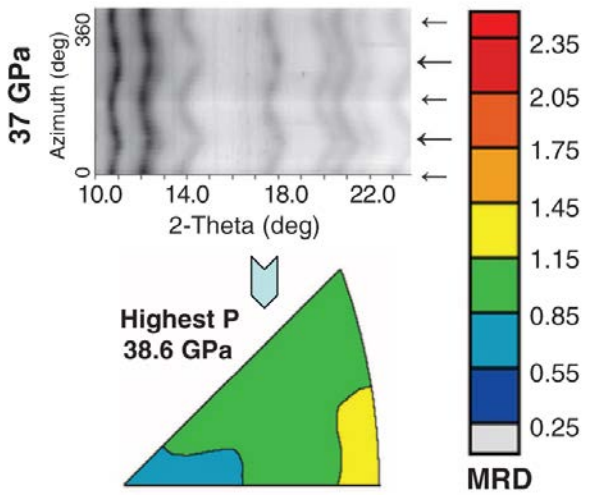


Figure 35. *Top left: Azimuthally (0-360°) "unrolled" diffraction image of nickel nanograins at 38 GPa. Long, thick arrows represent the maximum compression direction and short thin arrows represent the minimum compression direction. Curvatures in the diffraction lines indicate stress in the sample. The texture is evident through the systematic variations in intensity along the azimuth direction (bottom to top in the figure). Bottom left: The pole figure derived from the diffraction data shows texture development in the sample. Texture strength is expressed in terms of a multiple of the random distribution. MRD = 1 indicates a random distribution (no texture), and a higher MRD value, according to the scale bar at right, indicates a stronger texture.*

computer analysis, this critical limit would occur in nanocrystals at sizes between 10 and 30 nm. Now, advances in radial diffraction techniques with the DAC have allowed measurements on nanomaterials under stress and have paved the way for new types of analyses that will yield detailed information on a wide variety of samples at extreme conditions. **Chen** and co-workers were able to show that the activities of the structural irregularities that accompany deformation were occurring even in nickel nanocrystals 3 nm in size above 18.5 GPa. This result demonstrates that so-called dislocation-associated deformation is a function of both pressure and particle size, as previously thought, but also that the particle size can be smaller than computer modeling had anticipated. These findings help constrain the fundamental physics of deformation under pressure at the nanoscale and demonstrate the importance of the radial XRD technique for investigating these processes.[10]

2.5 Electronic and Magnetic Structure and Dynamics

Relationships between crystal structure and electronic and magnetic properties lie at the heart of understanding materials behavior at extreme conditions, and this data is key for many applications in stockpile stewardship. CDAC has pursued theoretical and experimental developments in this area, and efforts to improve both apparatus and methods for these types of studies are ongoing in many CDAC groups. Current measurement capabilities are now allowing and understanding of the physical properties of materials at the level of electrons, which is a fundamental requirement for not only understanding existing materials, but also for designing new materials.

Activation Volume for Polaron Hopping in Materials for Lithium Storage – Lithium-ion batteries have high specific energy, high specific power, and reasonable cycle life,[72, 73] and have had an enormous impact on computers and consumer electronics. Extending their service beyond power tools and consumer electronics, however, requires improvements in cost, safety, performance and lifetime. Many of these issues originate with the electrode materials for lithium storage. $LiFePO_4$ is a promising candidate material for cathodes of lithium ion batteries, with a relatively high capacity of 170 mAh/g and a high discharge voltage of 3.5 V vs. Li. Other important characteristics are that it is nontoxic, highly stable, and inexpensive. Unfortunately, the electron mobility in $LiFePO_4$ is a major technological concern because $LiFePO_4$ has the electronic structure of an insulator. Although conductive coatings are effective, there remains interest in improving its intrinsic conductivity.

The underlying mechanism of electrical conductivity in $LiFePO_4$ is known to be the motion of small polarons, which are the mobile electrons at Fe ions plus the distorted local environment around these ions. The local distortions are significant. The loss of an electron when an Fe^{2+} ion becomes an Fe^{3+} ion shortens the Fe-O bond distance by about 5%. Movement of a hole from the Fe^{3+} site to an adjacent Fe^{2+} site requires moving the local distortion, too. The charge and its distorted local environment, the small polaron, is mobile at higher temperatures when atomic vibrations bring

the local atomic structure of the adjacent site to a configuration compatible with bond distances and angles for an electron hop to an Fe^{3+} ion.

The mechanism of polaron hopping in $LiFePO_4$ is well suited for study with ^{57}Fe Mössbauer spectroscopy, which reveals several types of information about the nuclear environment of the resonant ^{57}Fe atoms, especially their valence. What is relevant to dynamics is that spectral features are broadened in energy, ΔE, when the charge is moving on the timescale of $t = h/\Delta E$. When valence electrons hop between Fe^{2+} and Fe^{3+} ions at a frequency of 10^7 Hz or higher, ΔE is comparable to the spectral energy differences of Fe^{2+} and Fe^{3+}, and the spectrum is distorted. This is seen in the conventional Mössbauer spectra in Fig. 36. At low temperatures the spectral signatures of Fe^{2+} and Fe^{3+} are distinct. At temperatures above 373 K, however, the spectral features change owing to charge hopping that occurs in times less than 100 ns. By measuring Mössbauer spectra at elevated temperatures, it is possible to determine the fractions of Fe atoms participating in polaron hopping, and determine the frequency for valence jumps. From these data, intrinsic electrical conductivities can be determined. The charge dynamics in a few Fe-bearing mixed-valence materials have been studied using Mössbauer spectrometry.[76-78] Nevertheless, rather little is known about how the thermal activation for polaron hopping in Li_xFePO_4 and other cathode materials are affected by material modifications, such as chemical composition or structure.

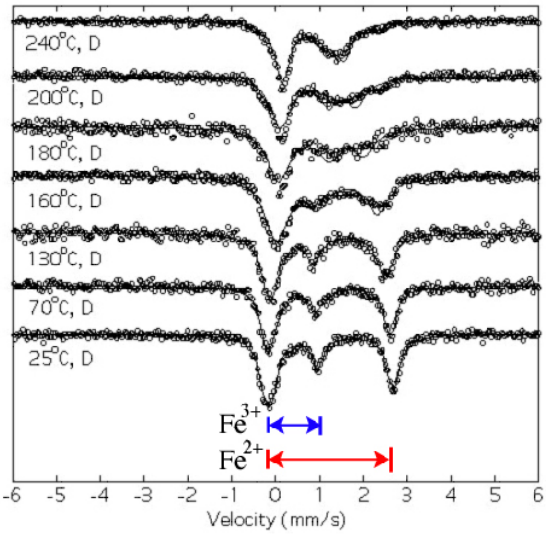


Figure 36 *Mössbauer spectra of the solid solution phase of olivine-structured $Li_{0.6}FePO_4$ at elevated temperatures,[74] showing well-resolved Fe^{2+} and Fe^{3+} doublets. Solid lines show fits from the hyperfine field distribution obtained by the method of LeCaer and Dubois.[75]*

Lisa Mauger and **Sally Tracy** in the **Fultz** group at **Caltech** have started novel measurements of the *activation volume* for small polaron hopping using nuclear forward scattering (NFS) at **HPCAT**. The activation volume is the change in volume of the material in the transition state during the polaron hop. A simple analysis shows what variables set the sign of ΔV, and how to extract it from experimental data.[79] Previous studies of activation volumes for small polaron hopping have been made by geophysicists on perovskite and olivine, using pressures from 1.2 to 40 GPa and temperatures from 200 to 700 K.[80-82] The activation volume was found to be small and negative for perovskite, although positive for olivine, and positive for $La_{2-x}Sr_xNiPO_4$.[83] A weakness of much of the previous work is that macroscopic bulk properties were measured, which are subject to effects of pressure on inter-crystalline interfaces, grain boundaries, and electrical contacts. Measurements by Mauger and Tracy of the activation volume for polaron hopping in $LiFePO_4$ were carried out at elevated pressures and temperatures.

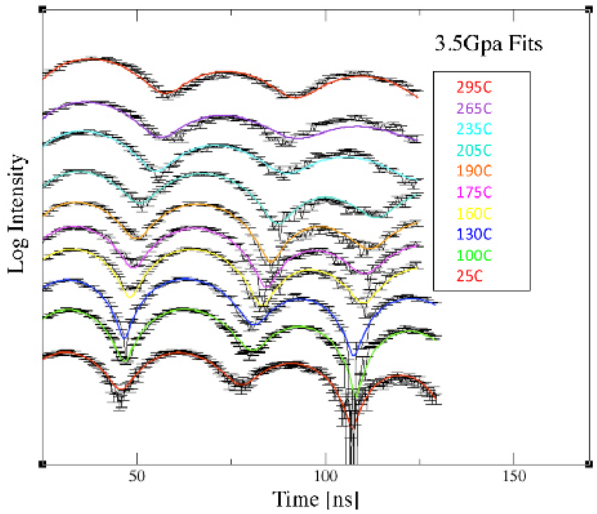


Figure 37. *NFS spectra of bulk $Li_{0.6}FePO_4$ at 3.5 GPa and various temperatures, overlaid with fits using CONUSS with the Blume model for hyperfine fluctuations.*

Some of the raw experimental results are shown in Fig. 37. These spectra for a sample at 3.5 GPa show that substantial changes do not occur until temperatures of perhaps 473 K, a higher temperature than for the control NFS spectra at 0 GPa (consistent with results from conventional Mössbauer spectroscopy). From this it is immediately apparent that the activation volume is a positive quantity for $LiFePO_4$, so pressure suppresses polaron hopping. From Arrhenius plots, the activation volume was found to be surprisingly large, almost 3 $Å^3$. Pressure is therefore a sensitive tool for altering charge dynamics in $LiFePO_4$. The Holstein model of polaron dynamics[84] predicts that the electron-phonon coupling is reduced with pressure, so other conductivity mechanisms may occur at higher pressures.

Magnetic Properties of Rare Earth Metals at High Pressure – The primary goal of the **Schilling** group at **Washington University** is to investigate in detail the mechanism(s) behind the pressure-induced volume collapse exhibited by many rare-earth metals. Possible mechanisms are: (1) Kondo volume collapse, (2) structure change due to *s-d* transfer, (3) valence change, and (4) Mott/Hubbard transition from 4*f* local to 4*f* band state. CDAC graduate student **Isaiah Lim** is currently carrying out electrical resistivity measurements on a dilute Y (0.5% Gd) alloy as a function of both temperature to 2 K and pressure exceeding 1 Mbar. Notable is that the pressure dependence of T_c to at least 80 GPa deviates very little from that of pure Y. If this trend continues to higher pressures, this implies that the mechanism responsible for the volume collapse in Gd metal at 60 GPa has nothing to do with its magnetic or valence state, but is likely the result of a structural transition due to simple *s-d* electron transfer. This result stands in marked contrast to what is observed for Ce or Pr impurities in La or Y hosts, which imply that in elemental Ce and Pr the volume collapse arises not primarily from *s-d* transfer but from the Kondo binding energy.

Graduate student **Gilberto Fabbris**, who is jointly supervised by **Schilling** at **Washington University** and **Daniel Haskel** at the **APS**, is focusing on elemental terbium (Tb), which undergoes a volume collapse of 5% at 53 GPa. Fabbris has carried out x-ray absorption near edge structure (XANES) and XES experiments on Tb metal to 70 GPa and finds neither a valence change over this pressure range nor a variation in the magnitude of the local magnetic moment on the Tb ion. Resistivity studies on Y (Tb) alloy reveal, however, that near 60 GPa a strong suppression of superconductivity in Y occurs, thus pointing to a Kondo mechanism as responsible for Tb's volume collapse, as for Ce and Pr, but in contrast to the *s-d* transfer mechanism in Gd.

Getting Serious with Cerium – Understanding f-electron elements has been an important problem in condensed matter physics for many decades. The challenges have involved developing a first-principles theoretical framework due to the fact that f electrons can exhibit either localized, highly correlated or itinerant behavior. In addition, f-elements are characterized by multiple low-energy states that make it difficult to correctly identify the ground state, a prerequisite for any theoretical method. Cerium under pressure has been a particular puzzle. It undergoes an isostructural volume collapse at 1.5 GPa at room temperature, a feature that has caused difficulties for existing models. The most serious discrepancy among competing models of f-electron behavior is the evolution of the magnetic moment of the Ce atom across the volume collapse transition. Therefore, a measurement of the magnetic moment with pressure should help validate one model over

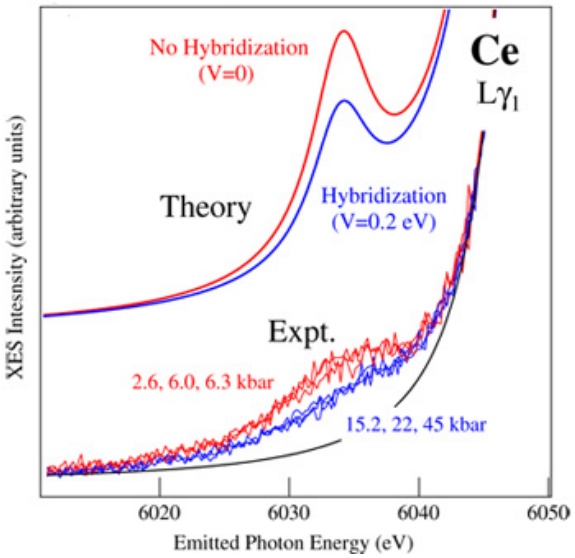


Figure 38. *X-ray emission spectrum of Ce metal in the region of the satellite shoulder on the main emission peak. Calculated spectra (top traces) show remarkable agreement with experimental results at low pressures (red) and above the transition pressure (blue).*

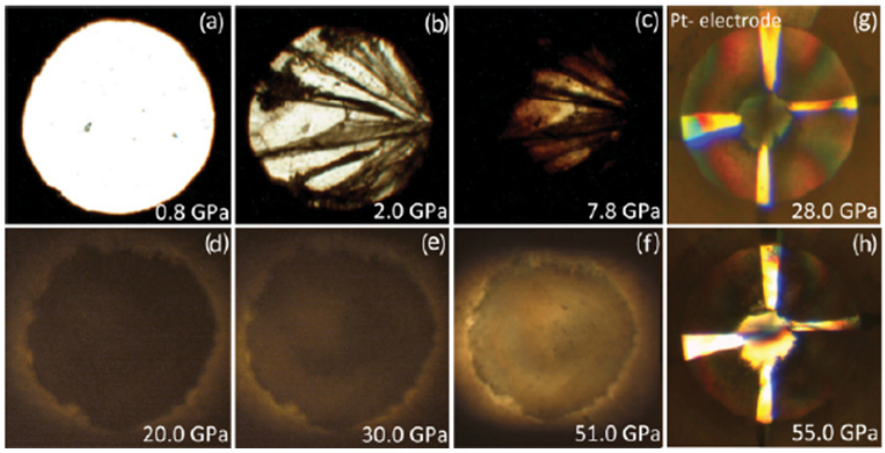


Figure 39. *Photomicrographs of CS_2 under high pressure showing its transformation from (a) transparent fluid to (b,c) molecular solid (Cmca) at ~1 GPa, to (d,e,g) black polymer above 10 GPa ((-S-(C=S)-)$_p$ or CS3), and eventually to (f,h) a highly reflecting extended solid above 48 GPa (CS4) at ambient temperature. The rightmost image (h) illustrates the metallic reflectivity of CS_2 samples above 55 GPa similar to those of Pt probes in a four-probe configuration for resistance measurements.*

others. Recently, a research group led by **Magnus Lipp** (**LLNL**), and including colleagues from **Stanford** and **Paul Chow** and **Yuming Xiao** from **HPCAT** carried out x-ray emission measurements on Ce metal up to 4.5 GPa designed to probe the magnetic moment. The key feature of the emission spectrum is the satellite shoulder on the main emission peak that represents interactions between 4f, 3d and 2p electrons in the atom (Fig. 38). The group showed that a theoretical model that explicitly accounts for the hybridization of 4f states with higher-lying conduction band states represents the physics correctly and produces excellent agreement between the experiment and the Kondo model of f-electron behavior as opposed to the Hubbard-Mott model. The approach adopted in this work will be relevant for other f-electron systems and will help expand the theoretical descriptions of this important class of materials.[85]

Highly Conducting Polymeric CS_2 – CDAC collaborator **Choong-shik Yoo** (**Washington State University**) has recently found experimental and theoretical evidence for the transformation of simple molecular carbon disulfide to an insulating black polymer with three-fold coordinated carbon atoms at 9 GPa, then to a semiconducting polymer above 30 GPa, and finally to a metallic solid above 50 GPa (Figure 39).[8] The metallic phase consists of a highly disordered three-dimensional network structure with four-fold coordinated carbon atoms at the carbon-sulfur distance of ~1.70Å, in plausible structures similar to those of extended phases of its chemical analog carbon dioxide. Carbon dioxide is an important terrestrial volatile often considered to exist in the deep interior of the Earth and may have strong implications for the deep carbon cycle.[86] This finding of highly disordered extended carbon disulfide showing high metallic conductivity, similar to that of elemental metals, is quite surprising, because the most "metallic" organic polymers exhibit barely metallic conductivity. In this regard, the origin of high metallic conductivity in this highly disordered, extended carbon disulfide phase is quite puzzling, and certainly deserves further experimental and theoretical studies on the exact nature of structural disorder and chemical bonding in this simple organic polymer. The **Washington State** group is now investigating this aspect of extended solids in an extended phase space as well as using chemical analogs. Beam time for this work at **HPCAT**

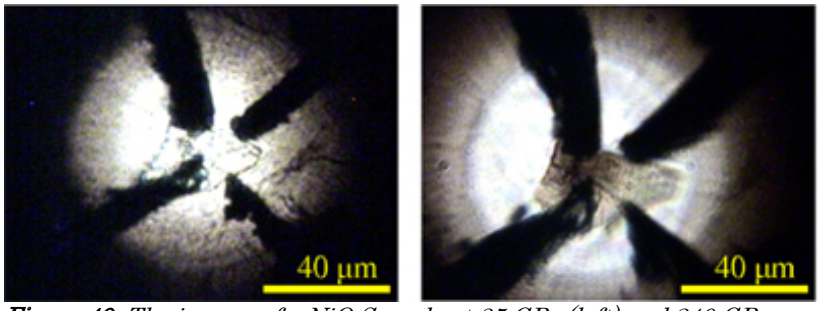


Figure 40. *The images of a NiO Sample at 35 GPa (left) and 240 GPa (right). The four Pt leads are connected to the NiO sample in the central part of the cBN gasket. At the transition pressure (240 GPa), the NiO sample becomes brown in color (semiconducting phase) and the metallic phase forms black percolation paths in the region of the highest pressure between the two electrodes (left). The cBN gasket is nearly transparent at these conditions.*

was provided by CDAC, and theoretical work was carried out in collaboration with **John Tse** at the **University of Saskatchewan**.

Elusive Metal Revealed – For decades, physicists have predicted that nickel oxide (NiO) would change from an insulator to a metal under compression, but their predictions had never been confirmed. Now, **Carnegie** scientist **Viktor Struzhkin** and colleagues from the **Russian Academy of Sciences** have discovered the conditions under which nickel oxide can turn into a conducting material. A 1 μm thick crystal was placed into a custom-designed DAC, with four thin foil leads to allow measurements of electrical resistance, which began decreasing at 130 GPa. At 240 GPa there was a dramatic, three-order-of-magnitude drop in resistance indicating the change from a semiconducting to a metallic state. The metallic part of the material was located in the region of highest compression (Fig. 40).[87]

Pressure-Induced Magnetic Transitions in Iron Carbides – In the **Li** group at **Michigan**, CDAC graduate student **Jiachao Liu** has investigated the structure, elasticity, and magnetism of the "Eckstrom-Adcock" carbide Fe_7C_3 up to Earth core pressures, using synchrotron-based single-crystal XRD and Mössbauer spectroscopy techniques. In these challenging experiments, two discontinuities in the compression curve were detected up to 167 GPa, the first of which corresponds to a magnetic collapse between 5.5 and 7.5 GPa and is attributed to a ferromagnetic to paramagnetic transition. At the second discontinuity near 53 GPa, Fe_7C_3 softens and exhibits Invar behavior, presumably caused by a high-spin to low-spin transition at Fe. In October 2012, XES and nuclear resonant inelastic x-ray scattering (NRIXS) spectra of compressed Fe_7C_3 were collected up to 145 GPa at **HPCAT**. The new data will allow elucidation of the nature of magnetic transitions in Fe_7C_3 under high pressure and determine the effect of the transitions on its density and sound velocities.

Insulator-Metal Transition and Colossal Magnetic Resistance in $LaMnO_3$ – Research carried out at **Carnegie** details the rich physics associated with how oxide materials transform from insulators to metals by application of pressure. Researchers from **Stanford** and **Carnegie** have provided the first experimental evidence for metallic $LaMnO_3$, formed when the Jahn-Teller distortion at Mn^{3+} is suppressed. Manganites have been widely investigated since the colossal magnetoresistance (CMR) effect was discovered at the insulator to metal transition. This effect promises new technical applications in the field of electronic and spintronic devices. Understanding,

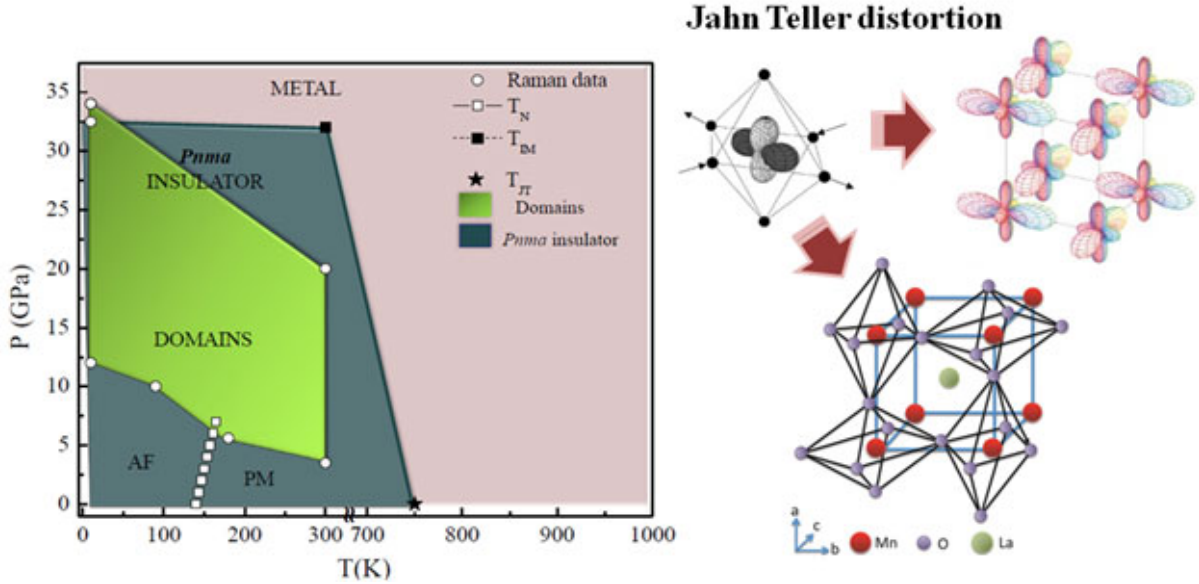


Figure 41. *Left: P-T phase diagram of $LaMnO_3$. Paramagnetic phase (PM), antiferromagnetic phase (AFM). Green area: P-T region with coexistence of domains. Dark blue area indicates the insulating P-T region. Right: Representation of the Jahn Teller distortion effects on the $LaMnO_3$ structure and orbital ordering.*

and ultimately controlling this effect, however, remains a challenge because of the number competing interactions.

$LaMnO_3$ is a very complex material due to the strong coupling between lattice, orbital, electronic, and spin degrees of freedom. High pressure-low temperature Raman spectroscopy measurements resolved the ongoing debate about the nature of the pressure-driven insulator-metal transition. This study provides the first experimental evidence for the persistence of the Jahn-Teller distortion within the insulating phase, and demonstrates that the insulator-metal transition is connected with the disappearance of the distortion. The formation of inhomogeneous domains – some with and some without distortion – was also observed in a wide region of the *P-T* phase diagram. The metallization process starts when the breakdown of undistorted to distorted octahedra (Fig. 41) hits a critical threshold in favor of the undistorted octahedra. In the recent years several theoretical and experimental studies related the CMR effect to the existence of inhomogeneous and competing states. Therefore, separation into domains opens up the possibility of inducing the CMR effect in undoped $LaMnO_3$ by applying pressure.[88]

Cool Crystals – A new and efficient way to pump heat using crystals has been discovered by Carnegie Summer Scholar **Maimon Rose (Chicago)** and **Carnegie's Ronald Cohen**. The crystals can pump or extract heat, even on the nanoscale, so they could be used on computer chips to prevent overheating or even meltdown, which is currently a major limit to higher computer speeds. The pair performed first-principles simulations on ferroelectric lithium niobate ($LiNbO_3$) and found that the introduction of an electric field causes a giant temperature change in the material, dubbed the electrocaloric effect. The electrocaloric effect pumps heat through changing temperature by way of an applied electric field. The effect has been known since the 1930s, but has not been previously exploited. Rose and Cohen found that the effect is larger if the ambient temperature is well above the transition temperature to the parraelectric state, so low transition temperature materials are preferred.[89]

Electronic Spin Transition of Iron in Phase D at High Pressure – CDAC graduate student **Yun-Yuan Chang (Northwestern)** has discovered a pressure-induced, electronic spin transition in iron in the dense hydrous magnesium silicate, phase D, using XES at HPCAT (Fig. 42). Among dense hydrous magnesium silicates potentially transporting water into Earth's deep interior, phase D ($MgSi_2H_2O_6$) exhibits the widest stability range extending into the lower mantle along very cold slab geotherms. Phase D contains nearly 12 wt% H_2O yet has a dense structure (r_0 = 3.3 g/cm^3) featuring Si in six-coordination with OH. Because subducted sediments in oceanic lithosphere include significant Fe and Al, the influence of these chemical substitutions on the structure and physical properties of phase D are under investigation, especially the possibility of pressure-induced spin transitions of Fe. Gem-quality single crystals of phase D that are rich in Fe^{3+} and Al were synthesized at 25 GPa and 1673 K with approximate composition: $MgSi_{1.5}Fe^{3+}_{0.15}Al_{0.3}H_{2.5}O_6$. Ferric iron occupies only octahedral sites in the

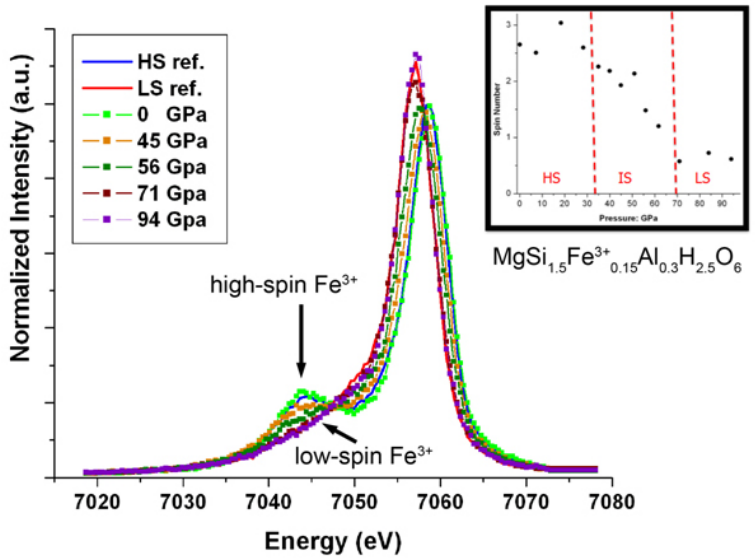


Figure 42. *XES measurements on $MgSi_{1.5}Fe^{3+}Al_{0.3}H_{2.5}O_6$ taken at HPCAT. The pressure-induced spin transition of $^{VI}Fe^{3+}$ occurs between 35 and 70 GPa, as indicated by the disappearance of the satellite peak at 7044 keV. Inset: Evolution of spin state (high, intermediate, low) with pressure.*

crystal, allowing isolation of the electronic spin transition of Fe^{3+} in octahedral coordination. XES measurements were carried out to 90 GPa at HPCAT. The experimental results reveal a gradual pressure-induced spin transition at Fe^{3+} between 35-70 GPa, which is also observed as a discontinuity in the compression curve. Because Fe^{3+} is isolated on one 6-coordinate site of this structure, results from this study are also useful in interpreting the nature of spin transitions in mixed-valence iron at multiple sites in other mantle phases such as silicate perovskite. This work was carried out in collaboration with CDAC Academic Partner **Jung-Fu Lin** (**UT-Austin**).

Superconductivity and Structure in FeSe – Magnetic elements such as iron typically do not exhibit superconductivity, and their magnetic nature has been considered incompatible with a state of zero electrical resistance, even at liquid helium temperatures. With the discovery in 2008 of the iron pnictide superconductors, however, a new set of problems concerned with the nature of the superconducting state has been under intense investigation. In particular, the iron-based superconductors have transition temperatures that are extremely sensitive to applied pressure, an observation that suggests a strong correlation between superconducting properties and crystal structure in these materials.

CDAC graduate student **Walter Uhoya** from **Alabama–Birmingham** and colleagues from **Illinois Wesleyan University**, the **Institute of Physics at Taipei** and **LLNL** have shown that designer diamond anvil technology developed for the measurement of electrical resistance can be used at a synchrotron source to perform simultaneous structural and electrical resistance measurements directly at high pressures and low temperatures (Fig. 43).

Uhoya performed the experiments on a sample of the compound $FeSe_{0.92}$ at pressures up to 74 GPa and temperatures down to 4 K at **HPCAT**. The results showed that the tetragonal phase present at ambient conditions transforms to an orthorhombic (*Cmma*) phase at ~ 90 K, which becomes superconducting at ~8.5 K. The superconducting T_c increases rapidly with pressure reaching a maximum of 28 K at ~6 GPa. Surprisingly, the maximum in T_c corresponds to an onset of a pressure-induced transition from the *Cmma* phase to the *Pbnm* phase reported concurrently at 6 GPa at low temperatures.

Above 6 GPa, T_c decreases gradually with increasing pressure, and disappears completely at 14.6 GPa, where the compound adopts the *Pbnm* phase. The gradual decrease in T_c between 6 and 14.6 GPa coincides with a gradual distortion of the $FeSe_4$ tetrahedral layers in a mixed phase region where *Cmma* and hexagonal $P6_3/mmc$ phases continuously transform to the *Pbnm* phase. **Uhoya** and his advisor, CDAC Partner **Yogesh Vohra,** have now documented the existence of four distinct phases in the *P-T* phase space investigated and have shown that superconductivity occurs only in the *Cmma* phase.[90]

The results and new methodology reported by the **Alabama–Birmingham** group are highly beneficial for ongoing studies aimed at understanding the phenomenon of high-temperature superconductivity and its response to crystallographic modulations under applied pressure.

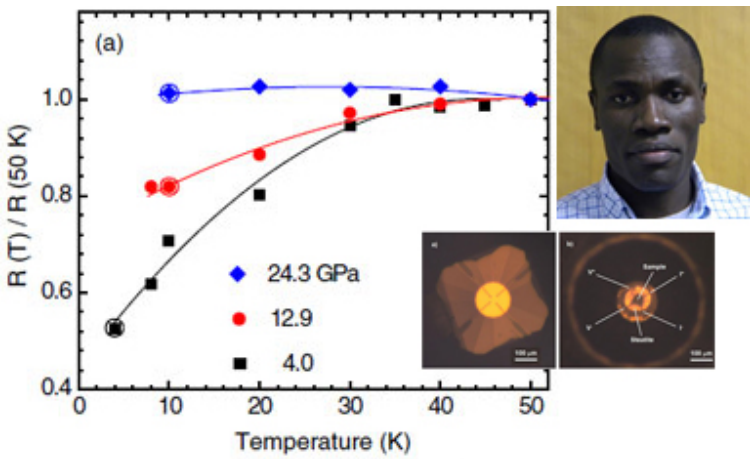


Figure 54 *Temperature dependence of electrical resistance for $FeSe_{0.92}$ measured using a designer DAC at HPCAT. XRD measurements were taken simultaneously with resistivity measurements at each P-T point. Inset: designer DAC for simultaneous superconductivity and structural measurements at high pressure. Top right: CDAC graduate student* ***Walter Uhoya*** *(**Alabama–Birmingham**).*

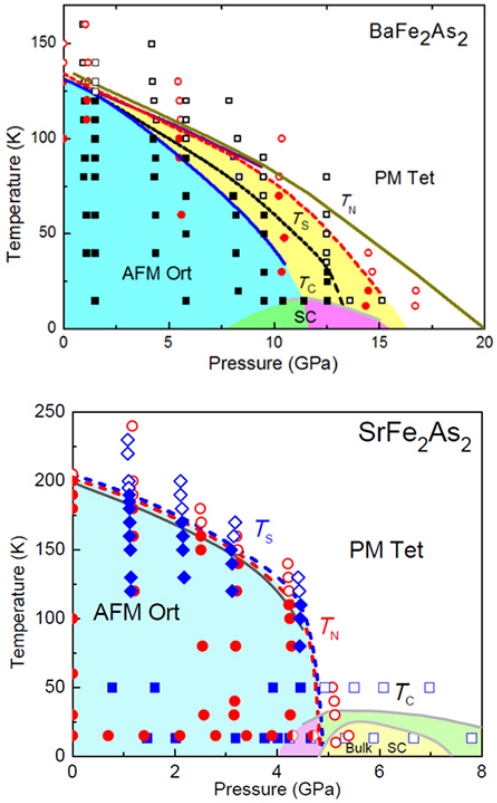


Figure. 44.*Schematic P-T phase diagram of $BaFe_2As_2$ (top) and $SrFe_2As_2$ (bottom), constructed using synchrotron x-ray diffraction and Mössbauer spectroscopy results.*

Iron-Based Superconductors at High Pressure and Low Temperature – At **UT-Austin**, the **Lin** group has performed a series of synchrotron x-ray spectroscopy experiments at the **APS** to investigate the interplay between structural, magnetic, and electronic transitions of the newly discovered iron-based high-T_c superconductors in a cryogenically-cooled DAC, focusing on the "122" iron pnictide (AFe_2As_2; A: Ba, Ca, Sr). The research goal is to apply extreme *P-T* conditions to determine dominant mechanisms responsible for the unconventional superconductivity occurring in the iron-arsenic layers of the system. These research projects are conducted at **HPCAT** by CDAC graduate student **Jin Liu.** Synchrotron Mössbauer and XRD are used to investigate structural and magnetic transitions of ferropnictide materials ($BaFe_2As_2$ and $SrFe_2As_2$) at high pressures and low temperatures. The results show that the structural and magnetic transitions occur quite differently in these two compounds. The transitions of $BaFe_2As_2$ are coupled at ~140 K at ambient pressure, but are substantially suppressed by increased pressure so that the onset of partial magnetic ordering occurs at a higher temperature than the structural distortion, whereas the complete occurrence of the antiferromagnetic state concurs with the orthorhombic phase (Fig. 44). On the other hand, the magnetic and structural transitions in $SrFe_2As_2$ are coupled together at high pressures and low temperatures. Current results support the local moment model involving the spin fluctuation and interaction as the major factor for the origin of superconductivity in pnictides.

Pressure Induced Superconductivity in $Ba_{0.5}Sr_{0.5}Fe_2As_2$ – Undoped iron-based pnictide compounds of the type AFe_2As_2 (A = divalent elements such as Ba, Sr, Ca and Eu) have been shown to become superconductors under high pressure.[91] Binary solid solution of the parent AFe_2As_2 (A= divalent alkaline earth elements) materials such as $Ba_xA_{1-x}Fe_2As_2$ (A=Sr, Ca, and Eu, $0 < x < 1$) may be promising as a new material platform for further investigation of the interplay between the crystal structure, magnetism, and superconductivity under high pressure, or chemical substitution, or both. However, such solid solutions of iron-pnictide compounds have presently not been investigated under high pressures. The **Alabama–Birmingham** group of **Yogesh Vohra** have been collaborating with **A. S. Sefat** of **ORNL** and **S. T. Weir** (**LLNL**) to investigate the electronic, structural and magnetic properties of such solid solutions under high pressure and low temperature

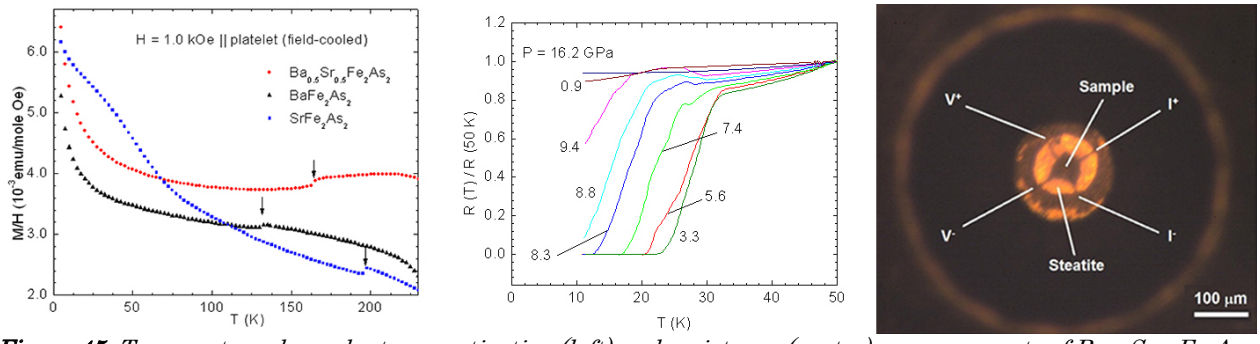


Figure 45. *Temperature dependent magnetization (left) and resistance (center) measurements of $Ba_{0.5}Sr_{0.5}Fe_2As_2$. Right figure is the Designer DAC used for high pressure superconductivity measurements.*

conditions. In this work, a series of temperature-dependent electrical resistance measurements at high pressure and down to 10 K have been undertaken on $Ba_{0.5}Sr_{0.5}Fe_2As_2$ along with preliminary measurements of the temperature-dependent magnetization and structural characteristics at ambient pressure.

The magnetization measurements at ambient pressure reveal the existence of AFM ordering of the Fe ion at 164 K (Fig.45, left). Additionally, the magnetization results on the $Ba_{0.5}Sr_{0.5}Fe_2As_2$ platelet at ambient pressure show no evidence for superconductivity down to 5 K, similar to the results on the parent compounds $BaFe_2As_2$ and $SrFe_2As_2$. The high-pressure electrical resistance measurements were performed on single crystal $Ba_{0.5}Sr_{0.5}Fe_2As_2$ platelets to pressures of 16 GPa and temperatures down to 10 K using designer diamond anvils under quasi-hydrostatic conditions with an insulating steatite pressure medium. The resistance measurements show evidence of pressure-induced superconductivity with an onset transition temperature at ~31 K and zero resistance at ~22 K for a pressure of 3.3 GPa (Fig. 45, center). The transition temperature decreases gradually with increasing pressure before completely disappearing for pressures above 12 GPa. The present results provide experimental evidence that a solid solution of two 122-type materials, *e.g.*, $Ba_{1-x}Sr_xFe_2As_2$ ($0 < x < 1$), can also exhibit superconductivity under high pressure. Further high pressure structural studies are scheduled to be performed at **HPCAT** (BM-D) in the coming months to fully understand this interconnection between the appearance/disappearance of superconductivity and the structural properties of the 122 materials under pressure. This work is part of the thesis project of CDAC graduate student **Walter Uhoya**.

Structure, Magnetism, and Superconductivity in $(Ca,Sr)Fe_2As_2$ – The ferropnictide superconductors provide a rich playground for investigating the interplay between structure, magnetism, and superconductivity.[92] At **LLNL**, **Jason Jeffries** has been studying the tetragonal, pseudobinary alloy $(Ca_{0.67}Sr_{0.33})Fe_2As_2$, which is unstable towards a concomitant magnetic and structural transition that occurs near 200 K, which then yields an antiferromagnetic, orthorhombic unit cell. Under pressure, the magnetostructural transition is suppressed to lower temperatures, but before the transition is driven to zero temperature, a new structural transition occurs. This new phase transition is an isostructural transition from the parent tetragonal cell to a collapsed tetragonal cell. The isostructural collapse is driven by the development of As-As bonding across the mirror plane of the crystal structure.[9]

Within the collapsed tetragonal phase, superconductivity develops with a maximum transition temperature near 22 K. Theoretical calculations suggest that increased As-As bonding drives a reduction in the Fe moment,[93] so the magnitude of the Fe moment in the collapsed phase is a critical component to evaluating the pairing mechanism for the observed superconductivity. Using XES under pressure at **HPCAT**, preliminary measurements of the Fe moment at room temperature reveal a continuous suppression of the moment up to 6 GPa. Previous results on $Ba(Fe,Co)_2As_2$ at ambient pressure show only a modest temperature dependence on the Fe

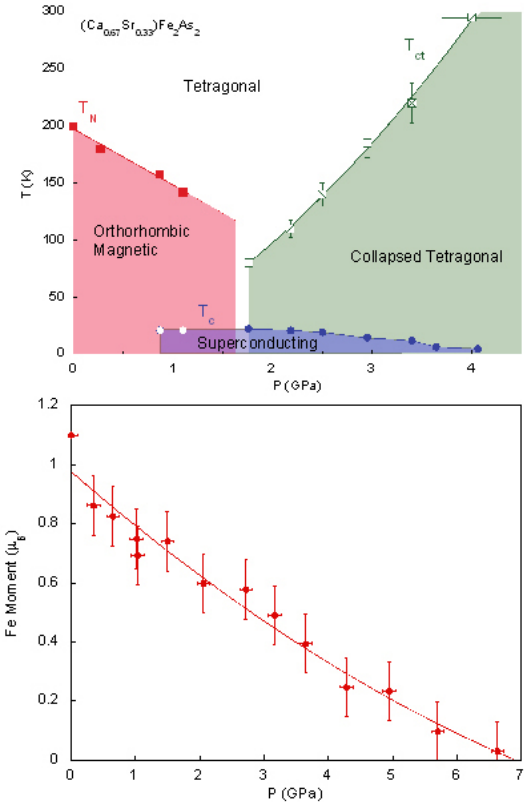


Figure 46. *Top: electronic/structural phase diagram of $(Ca_{0.67}Sr_{0.33})Fe_2As_2$. Bottom: pressure-dependent evolution of the Fe local moment extracted from XES experiments at the Fe Kβ line.*

moment.[94] Taken together, this would suggest that the observed superconductivity in the collapsed tetragonal phase of $(Ca_{0.67}Sr_{0.33})Fe_2As_2$ exists within a lattice of magnetic Fe ions. Recent experimental results are summarized in Fig. 46.

2.6 High *P-T* Chemistry

Completing the array of critical structure-property information on materials behavior is the compositional information provided by investigations in the area of high *P-T* chemistry. The wide variety of systems under study in CDAC groups continues to grow in importance as these studies reveal how sensitive are the physical and chemical properties of materials are to changes in composition, particularly at extreme conditions.

Fast Spectroscopy of Energetic Materials: Laser Shocked Self-Assembled Monolayers – The **Dlott** group at **Illinois** is investigating at the molecular level the very fast process known as energetic material (EM) "initiation," which is the point at which initially stable molecules begin to react. In these experiments, where the molecules are "pumped" by a shock (driven by a laser pulse) and "probed" by IR spectroscopy, the time resolution is usually limited by the shock transit time across the molecular layer. Such thin samples are difficult to probe on short time scales, but the group has developed the ability to obtain very high-quality vibrational spectra using a nonlinear coherent IR method known as "broadband multiplex vibrational sum-frequency generation spectroscopy with nonresonant background suppression" or SFG. The concept is outlined in Fig. 47.

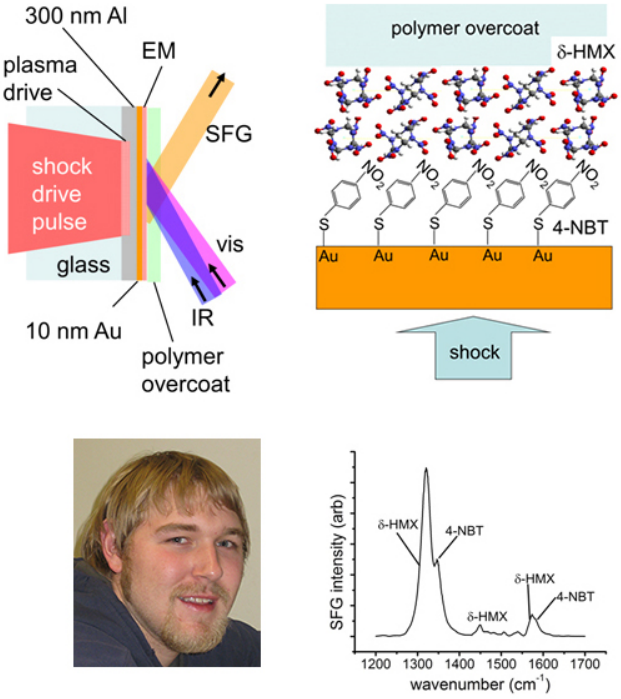


Figure 47. *Top left: Schematic of one element of a shock target array for ultrafast shock vibrational spectroscopy of ultrathin molecular layers. Top right: A sample configuration with a nitro self-assembled monolayer (SAM) with a few nanometers of δ-HMX. Bottom left: SFG spectrum in the nitro stretch region, from shock target array with 4-nitrobenzenethiol (4-NBT) monolayer and 5 nm of HMX. Bottom right: CDAC graduate student* ***Chris Berg*** *(**Illinois**).*

The molecular layers are grown or deposited on a metal thin film, usually Au, and they are confined with a few-micron thick polymer layer. Experiments are repeated at 10-100 Hz and thousands of shots accumulated by rastering a large-area (25 cm^2) sample with a motorized translation stage. Also shown in Fig. 47 is a two-component sample invented by CDAC student **Chris Berg.** The first component is a highly-ordered self-assembled monolayer (SAM) of 4-nitro-benzenethiol. SFG probes the symmetric and antisymmetric nitro stretches of this layer. The second component is a deposited layer of HMX (5 nm thick) that appears to be in a form close to the δ-HMX crystal since it is clearly noncentrosymmetric and its spectrum closely resembles δ-HMX standard samples. With the SFG technique, it is possible to simultaneously probe nitro stretches of both components as shown in Fig. 47. The quality of the spectra in which appear to have come from a conventional IR or Raman spectrometer, is remarkable given that they were obtained with 1 ps time resolution on a layer <5 nm thick.

In order to interpret such spectra, they are compared to spectra obtained at static high temperature and pressure. This means high pressure spectra of monolayers in the DAC need to be obtained. To realize this goal, CDAC student **Kathryn Brown** invented a tiny photonic chip that can be inserted into a DAC sample chamber that amplifies the Raman spectra by $10^5 – 10^6$ using surface-enhanced Raman scattering.

Fast Spectroscopy of Energetic Materials: Flyer Plate Nanosecond Spectroscopy – The Dlott group has also developed a convenient source for impact shock experiments that is conveniently synchronized with ultrafast spectroscopy instrumentation, that has enough kinetic energy to create substantial shock compression (~10 GPa or more) and enough energy to initiate common energetic materials (Fig. 48). The criteria for initiating an energetic material is that P^2t must exceed a critical value, so rather high pressures are needed with short-duration shocks. The goal for studies of chemical systems is a shock duration of 10-20 ns and an impact velocity up to 5 km/s. The achievable pressure in a typical molecular medium such as PMMA with a 5 km/s impact from an Al flyer is ~30 GPa.

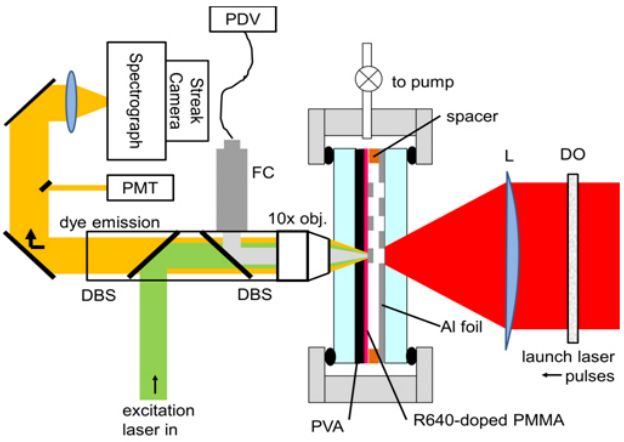


Figure 48 *Schematic of launch apparatus, sample, probe and detectors. The sample consists of a glass window with a 30 μm PVA cushion layer and an 8 μm layer of PMMA doped with R640 dye aggregates. The polychromatic probe transmits and receives returned 1.55 μm light from the photonic Doppler velocimeter (PDV). It transmits 527 nm light from the excitation laser and receives returned visible emission. Key: 10x obj = 10X microscope objective; DO = diffractive optic; L = aspheric objective lens; DBS = dichroic beam splitter; PMT = photomultiplier tube; FC = fiberoptic collimator.*

In one example of high-speed spectroscopy, from the work of **Kathryn Brown** and **Will Shaw**, Rhodamine 640 dye is dissolved in PMMA. A 25 mm flyer plate impacts a 40 mm thick PMMA layer. DISAR data (Fig. 49) show that the collision occurs at ~83 ns, where velocity drops to 1.05 km/s, so 1.05 km/s is the material velocity U_p in PMMA. There is a subsequent ~8 ns period of steady shock loading. Recently, Hugoniot measurements were made on this solvent-cast PMMA material.[95] The results gave good agreement with PMMA data from the LASL database. For a material velocity U_p = 1.05 km/s, the shock velocity U_s = 4.2 km/s, the compression is DV/V = 0.25 and the shock pressure P = 5.2 GPa. At the peak of shock compression, there is considerable extra blue-edge (hot-band) intensity. As the shock unloads, there is reduced blue-edge intensity but it is still more than in the unshocked material. The blue-edge hot-band emission is indicative of the net temperature increase caused by shock compression. Thus it is possible to use the R640 dye as both an internal spectroscopic pressure and temperature gauge.

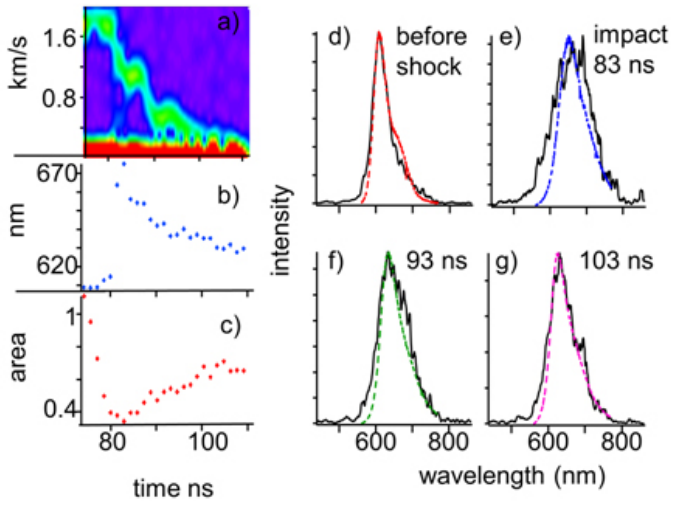


Figure 49. *(a) Blow-up of velocity history during flyer collision with PMMA showing how the incoming 1.6 km/s flyer slows to 1.05 km/s in contact with PMMA. (b) and (c) Time-dependent peak shift and intensity of R640 dye emission. (d)-(g) transient emission spectra compared with static HP spectra from a diamond anvil cell. The peak redshift indicates higher pressures. Extra intensity on the blue edge (hot-band emission) indicates higher temperatures.*

In the most recent measurements, samples are thin enough so that the shock transit time across them is a few nanoseconds, so the emission burst can provide intrinsic physical and chemical information. Figure 50 shows data on Al/Teflon where the Al thickness is 50 nm and the Teflon thickness is 3 mm. At 3 km/s there is an

emission burst from Teflon only lasting ~100 ns. When Al is added, the burst becomes much more intense and it develops a two-part structure. Insight into the mechanism comes from emission spectra from Teflon alone. The emission at lower flyer velocities shows bands characteristic of C_2 emission (Swan bands). If there is C_2 present, then there is also gaseous fluorine, which suggests that the impact decomposes Teflon and the fluorine gas then attacks the Al through its passivating oxide layer. The first emission burst is caused by the results of this attack. Subsequently the remaining material, especially the interiors of the Al particles, starts to burn, giving rise to the second burst. This mechanism is in stark contrast to our previous studies of flash-heating of Al/Teflon. Flash heating vaporizes the Al leaving Teflon cold, so reactions occur when Al plasma attacks Teflon.[95-97]

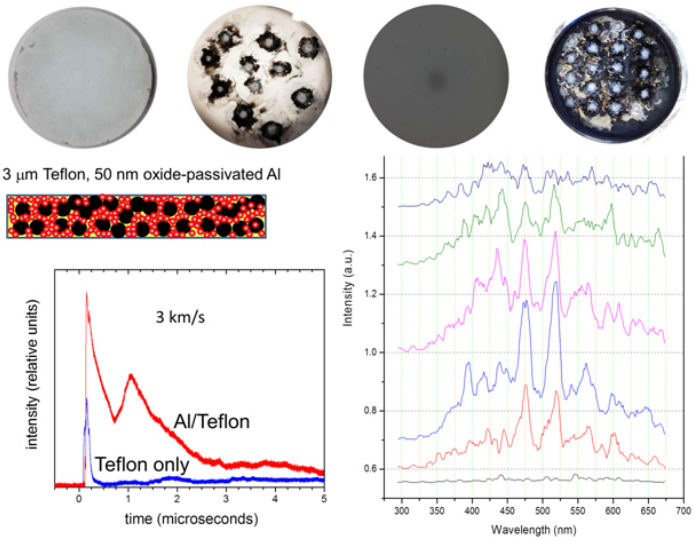


Figure 50. *Al/Teflon samples (right to left), Teflon only before and after flyer impact; Al + Teflon before and after flyer impact. The emission burst from Teflon with 3 km/s impact lasts about 100 ns. A brighter, longer-lived signal with a two-burst structure is observed with Al/Teflon. The emission spectra with 0.76 km/s impact on Teflon only show clearly resolved C_2 Swan bands, indicating that Teflon decomposes into carbon and fluorine.*

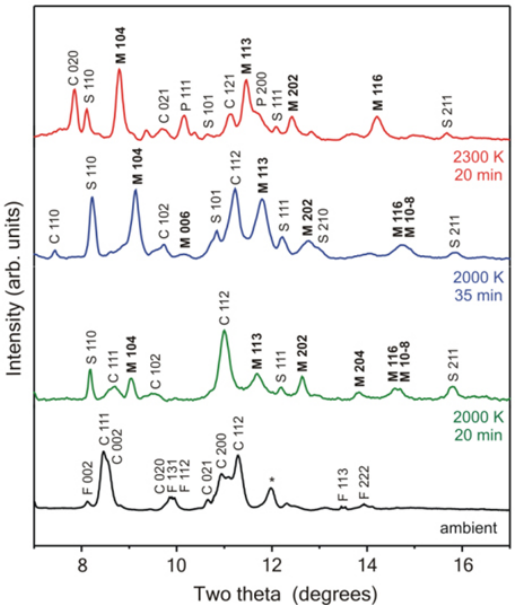


Figure 51. *X-ray diffraction patterns collected before heating (ambient), after 20 and 35 min of heating at ~2000 K, and after 20 min of heating at ~2300 K. M= magnesite, S=stishovite, F=forsterite, P=periclase, C=solid CO_2. The CO_2 at ambient temperature is CO_2-III (Cmca); CO_2 at 2000 K is CO_2-IV ($P4_12_12$); CO_2 at 2300 K is CO_2-IV (Pbcn). The presence of CO_2 peaks throughout the experiment indicates a solid-state reaction. The asterisk (*) indicates contribution from the gasket.*

Magnesite Formation in Earth's Mantle –
Magnesite ($MgCO_3$) is regarded as the primary carbon-bearing mineral in Earth's mantle, where its stability has been verified both experimentally[98, 99] and computationally.[100, 101] However, formation of magnesite at mantle conditions has not been investigated, despite the discovery of free CO_2 in mantle xenoliths from depths as great as 270 km.[102] The research has shown that magnesite can form at a variety of mantle conditions according to the reaction:

$$Mg_2SiO_4\ (s) + 2\ CO_2\ (aq) = 2\ MgCO_3\ (s) + SiO_2\ (s) \quad (1)$$

Since Mg_2SiO_4 is abundant in the mantle as forsterite, wadsleyite and ringwoodite, this reaction is likely to occur in the mantle. CDAC graduate student **J. McLain Pray** from **Michigan** used the laser-heated diamond-anvil cell and carried out synchrotron powder XRD experiments at **HPCAT**, supplemented by Raman spectroscopy, on samples gas-loaded with CO_2 as the pressure medium. He has also extended the investigation of reaction (1) by analyzing the starting olivine compositions from Fo90, $(Mg_{0.9},Fe_{0.1})_2SiO_4$, to Fo50 and Fo75, using both natural and synthetic olivine powders, and studied reaction (1) over a much wider pressure range at temperatures typical for the mantle. Magnesite formation was observed from 7 GPa to 30 GPa for all sample compositions along with stishovite (Figure

51). Above 10 GPa, CO_2 diffraction maxima were present throughout the experiment, indicating a solid-state reaction

A new finding is the apparent formation of separate carbonate phases, delineated by slightly offset Bragg peaks. Carbonate peaks show consistent shoulders on the lower 2θ-value side. This can be explained by the ionic ratio of Fe^{2+} relative to Mg^{2+}, resulting in larger unit cell parameter for the Fe-rich composition as compared with the Mg-rich sample. Additionally, the strong peak at 2θ = 6.5° is characteristic of Fe-rich carbonate and not Mg-rich carbonate. Since the olivine reactant had a 9:1 Mg:Fe ratio, a strong peak at 2θ = 6.5° would not be expected if the carbonate product maintained the same ratio, suggesting instead that a Fe-rich phase formed separately from the Mg-rich phase.

The suggestion of separate carbonate phase formation at elevated pressure is in contrast to several experimental studies that have found the Mg/Fe/Ca carbonate series to have a complete solid-solution. It should be noted, however, that previous studies have only exposed *pre-formed* carbonates to limited pressures up to 6 GPa. Thus it may be possible that formation of separate phases may indeed be thermodynamically favored during carbonate synthesis at elevated pressure and temperature, but that the formation of a single phase may be kinetically inhibited.

Low-Temperature IR-Reflectivity of Methane and Ethane – Light hydrocarbons such as methane (CH_4) and ethane (C_2H_6) are among the most important energy resources today. Knowledge of hydrocarbon properties and phase stability has applications ranging from stockpile stewardship to identifying states of CH_4 and C_2H_6 on icy bodies of the outer solar system. At **Northwestern University**, graduate student **Kimberly Adams**, along with faculty member **Steve Jacobsen** are collaborating with **Carnegie's Zhenxian Liu** and **Maddury Somayazulu** to study the low-temperature IR-reflectivity of methane and ethane across liquid-solid phase changes. By examining broad-spectrum IR-reflectance at NSLS Beamline U2A, changes in hydrocarbon phase states are identified more readily than with typical IR-absorption spectroscopy. Similar to methane, new measurements on ethane reveal a dramatic darkening of C_2H_6 upon melting at ~85 K (Fig. 52), which may help to explain the dark, lake-like features on the surface of Titan at 5 μm.

Hydrogen-Loaded Hydroquinone Clathrate – Clathrate compounds consist of molecules that form "host" structures, trapping appropriately sized "guest" molecules. Understanding the basic chemical interactions in these compounds is important over a broad range of areas spanning energy storage and pharmaceutical development. At **Carnegie**, **Timothy Strobel** and **CDAC** intern **Viktor Rozsa** (**Hillsdale College**) have recently discovered extremely novel behavior in hydrogen-loaded hydroquinone (ß-HQ-H_2) clathrate under pressure. While the vast majority of materials contract under hydrostatic compression, the volume of b-HQ-H_2 clathrate actually expands nearly 1% when compressed between 2.5 and 3.0 GPa. Over this pressure range, the negative bulk modulus and negative linear compressibility along the *a* and *b* axes are a consequence of a change in hydrogen occupancy from one to three molecules in the structure.

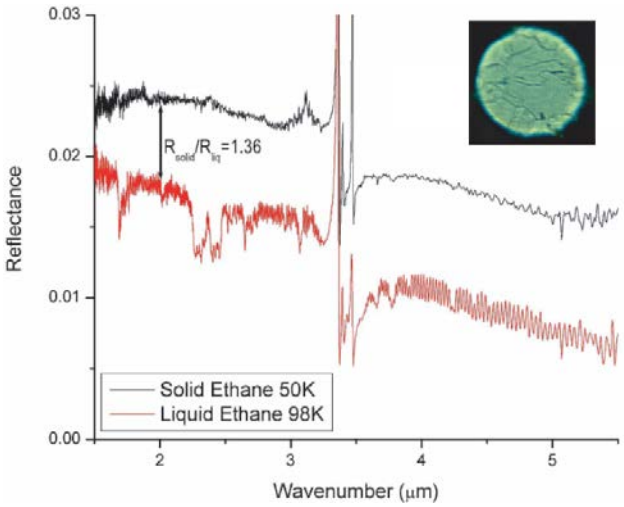


Figure 52 *Broad-spectrum IR-reflectance of C_2H_6 shows dramatic darkening upon melting at ~85 K, which may be used to help identify phase states of hydrocarbons on distant satellites in the solar system, such as Titan, which has a window of atmospheric transparency at 5 μm. Inset, crystallization of ethane is depicted at ~85 K on cooling.*

Hydroquinone (HQ), or quinol (1,4-benzenediol), has three known crystalline modifications: a, ß, and g. The ß phase is a clathrate structure trapping small molecules less than ~4 Å. ß-HQ-H_2

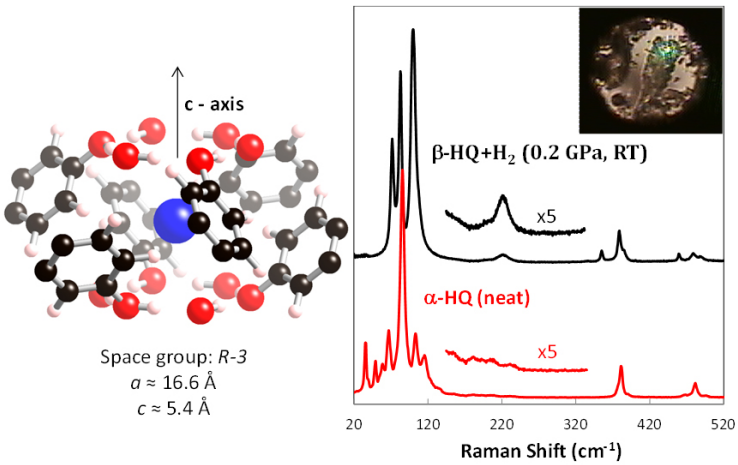


Figure 53. *Left: structure of b-HQ-H_2 clathrate cage with H_2 molecule inserted at the cage center (blue sphere). Right: Raman spectra of a and b modifications showing successful conversion to b phase after synthesis procedure. The out-of-plane bending mode at ca. 220 cm^{-1} and low-frequency libration modes (<120 cm^{-1}) are diagnostic of b-HQ clathrate. The inset shows a picture of loaded diamond cell.*

clathrate was synthesized by pressurizing finely ground a-HQ (~20 mm grains) with hydrogen at ~0.2 GPa in a DAC. The cell was heated at 340 K for eight hours to achieve 100% conversion to the ß phase. The ß-HQ clathrate cavities consist of six HQ molecules with $[OH]_6$ rings terminating the top and bottom of the cage along the *c* axis and benzene rings comprising the cage equator in the *a-b* plane. Figure 53 shows the structure of ß-HQ-H_2 clathrate and Raman spectra indicating successful synthesis.

Synchrotron powder XRD measurements were performed on b-HQ-H_2 clathrate in excess hydrogen up to 6 GPa at **HPCAT**. Diffraction patterns were indexed and refined to the *R-3* structure over the entire pressure interval, indicating no structural phase transitions Between 0.2 to 6 GPa, the *c* axis decreased monotonically by about 14%, while the *a* axis initially decreased by 0.5% up to 1.4 GPa, remained flat between 1.4 to 2.4 GPa, increased 1% between 2.4 to 3 GPa, and finally decreased by 1.3% between 3 and 6 GPa. This behavior was reproduced between two independent samples and was completely reversible with decreasing pressure.

Low pressure (<1 GPa) measurements are in excellent agreement with previous studies, showing a single vibron for singly occupied H_2, which is substantially red-shifted (-50 cm^{-1}) from bulk hydrogen. With increasing pressure, the hydrogen vibron "jumps" to higher frequency at *ca.* 1.4 GPa, concomitant with the flattening of the *a* axis compression in the diffraction measurements, and a more repulsive local environment for H_2. This behavior is attributed to the incorporation of a second H_2 molecule within the ß-HQ clathrate cage. Increased repulsion between the two molecules accounts for the shift in the vibron frequency, and the presence of a second molecule inside the cage explains the decreased compressibility of the *a* axis starting at 1.4 GPa. At pressures above 3 GPa a second "jump" and splitting for the vibron due to enclathrated H_2 is observed, with peaks that are blue-shifted from the bulk fluid phase. These features are attributed to the onset of triple occupancy of H_2, with two molecules located inside the HQ cage and one molecule located inside the center of the $[OH]_6$ ring at the top and bottom of each cage. The splitting of the H_2 vibron is accounted for by the different local H_2 environments, both of which are increasingly repulsive compared with the lower occupancy cases. Additionally, the onset of $[OH]_6$ ring occupancy explains the sudden increase in the a axis of the crystal (and volume increase) as H_2 molecules are

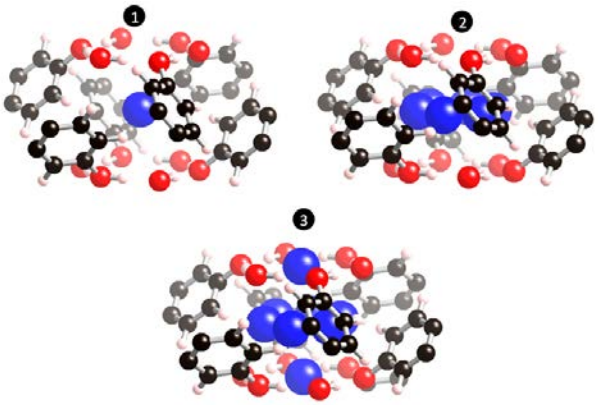


Figure 54. *Occupancy progression in b-HQ-H_2 clathrate. (1) <1.4 GPa, single occupancy; (2) 1.4 to 2.4 GPa, double occupancy; (3) >2.4 GPa, triple occupancy: 2 H_2 per cage, 1 H_2 per ring. For the double occupancy case, H_2 molecules are likely distributed between six equivalent sites in the cage center.*

forced into this site, expanding the cavity in the *ab* plane. Figure 54 summarizes the progression from single to triple occupancy in b-HQ-H_2 clathrate. This occupancy pattern is supported by recent molecular dynamics simulations.[103]

The increase in occupancy from one to three hydrogen molecules provides insights into the design of novel molecular hydrogen storage materials with higher hydrogen capacity and the unusual negative compressibility might provide clues towards the design of novel materials with advanced properties.

Heterogeneity in the Dynamics of Methanol – The glass transition has been the subject of extensive experimental and theoretical studies for many years, both for its fundamental interest and for its practical importance. Methanol, the simplest alcohol, is widely used in industry and research, and is a glass forming fragile liquid, which should be described by the Vogel–Fulcher–Tammann (VFT) equation. Mode coupling theory (MCT) further states that the dynamical properties of a fragile liquid are governed by a slow α-relaxation with strong temperature dependence and a fast β-relaxation that varies weakly with temperature. One of the predictions of MCT theory is that α-relaxation will diverge from β-relaxation toward the glass transition point and will rest at near glass transition temperature T_g.. The dynamical behavior of this glass forming liquid has been extensively studied, with the large majority of work focusing on the temperature evolution. Density favors the formation of fragile liquid and so in its compressed state methanol is predicted to be a fragile liquid also. In a study carried out at **Carnegie** by summer intern **Louis Loubeyre** from the **University of Paris VII** and his mentor **Muhtar Ahart**, Brillouin and Raman measurements were performed on methanol up to 10 GPa to study the evolution of dynamical properties toward the glass transition.

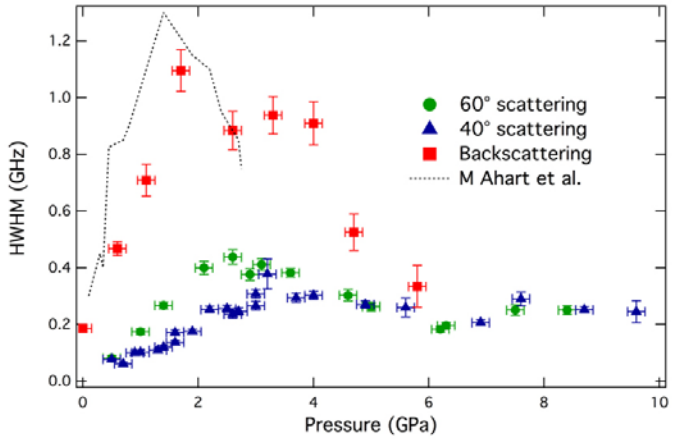


Figure 55. *Pressure dependencies of the linewidth of the LA mode measured at different scattering angles. The symbols dots, triangles and square represent respectively measurements in the 60°, 40° and backscattering geometries, respectively. The dashed line indicates previous measurements.*

The linewidth of the longitudinal acoustic mode shows a broad peak centered around 3 GPa, which defines the onset of the unrelaxed regime (Fig. 55), as determined using the well-established viscoelastic theory and a Vinet fit for the EOS. The pressure evolution of the relaxation time in the GHz range therefore may be obtained. Raman data are analyzed in terms of the Boson peak and its associated relaxation time in the THz range. The pressure evolution of these two relaxation processes complete previous determinations of relaxations at lower frequency based on dielectric measurements in super-cooled methanol. Relaxation processes in glass-forming methanol are now obtained over a wide frequency range.

Magnesium Oxide: From Earth to Super-Earth – The mantles of Earth and other rocky planets are rich in magnesium and oxygen. Due to its simplicity, the mineral magnesium oxide also happens to be a good model for studying the nature of planetary interiors. **Carnegie**'s **Stewart McWilliams** and colleagues from **LLNL** and **Berkeley**, including CDAC Steering Committee Member **Rip Collins** (**LLNL**), former CDAC Partner **Raymond Jeanloz** (**Berkeley**) studied how magnesium oxide behaves under the extreme conditions deep within planets . The work provides evidence that alters the current understanding of planetary evolution. Magnesium oxide is particularly resistant to changes when under intense pressures and temperatures. Theoretical predictions claim that it has just three unique states at the conditions of planetary interiors: solid under ambient conditions (such

as on the Earth's surface), liquid at high temperatures, and another structure of the solid at high pressure, which has never been observed in nature or in experiments on this material.[4]

The group observed magnesium oxide between pressures of about 300 GPa and then up to 1400 GPa and temperatures reaching as high as 50,000 K, conditions that range from those at the center of our Earth to those of larger exoplanets and super-Earths. Observations indicate substantial changes in chemical bonding as the magnesium oxide responds to these various external conditions, including transformation to a new high-pressure solid phase. This pioneering study takes advantage of new laser techniques to explore the nature of the materials that comprise the wide array of planets being discovered outside of our solar system. These methods allow investigations of the behavior of these materials at pressures and temperatures never before explored experimentally. In fact, there are indications that, when melting, magnesium oxide changes from an electrically insulating material to a metal similar to iron. Drawing from these and other recent observations, the it is concluded that while magnesium oxide is solid and non-conductive under conditions found on Earth in the present day, the early Earth's magma ocean might first been able to generate a magnetic field. Likewise, this metallic, liquid phase can exist today in the deep mantles of super-Earth planets, as can the newly observed solid phase.

Polymers at Extreme Pressures – Information on the behavior of polymers at high pressure cannot be obtained using conventional XRD techniques, due to the lack of long-range order in the material. Such information, however, is becoming increasingly important due to the key role of polymeric materials in a number of modern technologies. An example is the behavior of polymer-bonded explosives (PBXs); an improved knowledge of the properties of PBXs at peak pressures is key to optimizing their use in real applications. At Carnegie, Summer Scholar **Ari Benjamin (Williams College)** and Research Scientist **Muhtar Ahart**, along with collaborators from **LANL** applied Brillouin scattering techniques to investigating polymer behavior at high pressure, and succeeded in measuring the acoustic properties of KelF-800 to 85 GPa. Using information on the pressure evolution of longitudinal and transverse acoustic modes, the group was able to determine a full range of elastic properties for KelF-800. These challenging experiments yielded data on the C_{11} and C_{12} modulii, bulk, shear and Young's modulii, as well as the density of the material with pressure, which allowed a determination of the EOS.

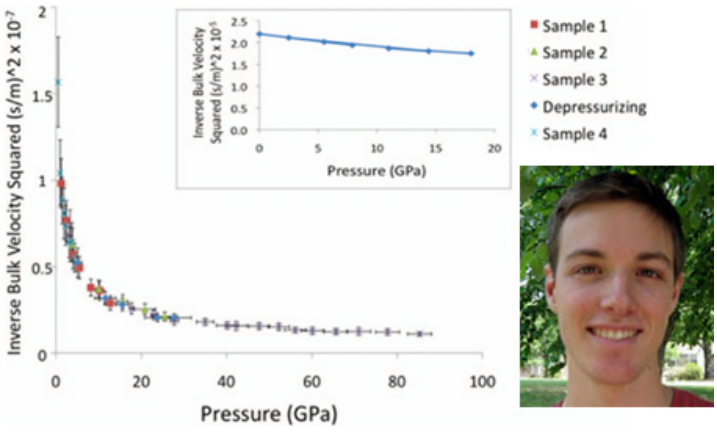


Figure 56. *Inverse bulk sound velocities squared for KelF-800 as a function of pressure. Inset: Inverse bulk sound velocity squared for MgO, a conventional crystalline solid, up to 20 GPa. Right: CDAC Summer Scholar* ***Ari Benjamin (Williams College)****.*

Previous investigations on polymeric materials had only reached 20 GPa, so the current work provides new insights on the behavior of polymers at very high compression. The results of the current work show that, over the pressure range up to 85 GPa, data on KelF-800 is best described in two separate pressure regimes, which correspond to the material before and after the collapse of the free volume (Fig. 56). Prior to the collapse of free volume, most polymers will behave similarly, but at higher pressures, after the collapse of the free volume, polymers will tend to behave much more like conventional crystalline solids.[7]

Probing Hydrogen above 300 GPa – Even though hydrogen is the most abundant element in the universe, an understanding of its properties under extreme pressure and temperature conditions

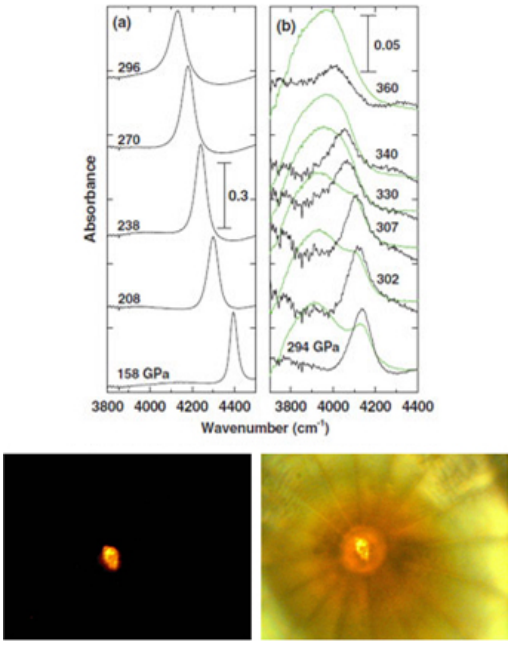


Figure 57. *Top: Representative synchrotron IR spectra of hydrogen in the region of the vibron (H_2 stretching mode) at selected pressures and 80 K. Bottom: Photographs of a hydrogen sample at 360 GPa and room temperature in a diamond anvil cell in transmission mode only (left) and both reflection and transmission mode (right).*

is not yet complete. Ultimately, the fundamental physics behind the behavior of this seemingly simple element can inform and expand our understanding of matter as a whole. New work from **Carnegie** scientists has enabled an examination of hydrogen under static *P-T* conditions not possible previously.[6] Theory has predicted a variety of novel states for hydrogen at high pressure, including the existence of room-temperature superconductivity and a fluid, or even superfluid, ground state. The interplay between theory and experiment has provided stringent tests for theoretical models and computational methods and has made the study of this material a problem of the first rank in condensed matter physics for nearly 80 years. Experimentally, work on hydrogen presents numerous challenges associated with confining the diatomic molecular form under pressure in a DAC. With continuous advances in technique, new findings in the multimegabar pressure range continue to push the limits of current models for its behavior.

The **Carnegie** team of **Chang-Sheng Zha**, **Zhenxian Liu**, and **Russell Hemley** were able to reach pressures of 360 GPa from 12 K to close to room temperature. Synchrotron IR spectroscopy was carried out at beamline U2A at the **NSLS**, **Brookhaven National Laboratory** (**BNL**). Measurements probed the transmission properties of hydrogen in order to look for the breakdown of the molecules to form the monoatomic and perhaps metallic state. The key signature of molecular hydrogen, the intramolecular vibration or vibron, persisted to the highest pressures achieved in the experiment, while the sample remained transparent in the near to mid-IR range (Fig. 57). The results indicate that the material is semiconducting, and possibly semimetallic, at these high *P-T* conditions.

The strong transmission of hydrogen in the mid-IR range contradicts a recent claim that the metallic state of hydrogen was reached below 300 GPa in DAC experiments. Meanwhile, a team from the **University of Edinburgh** and including **Carnegie's Alexander Goncharov** reports evidence for another phase of molecular hydrogen (near 220 GPa at 300 K). This work focused on a higher temperature range and somewhat lower pressures, and did not measure the metallic properties. Their work suggests that the structure of hydrogen in this new phase is a honeycomb made of six-atom rings, similar to the elemental carbon structure known as graphene.[104]

Super-Dense Aluminum from Ultrafast Micro-Explosions – Aluminum adopts a fcc structure at ambient conditions, but theoretical calculations have predicted possible phase transitions of fcc to hcp, and hcp to bcc at pressures of 120 GPa to 380 GPa, respectively. Up to now, however, only the first transition has been observed experimentally. An international research team including **Wenge Yang**

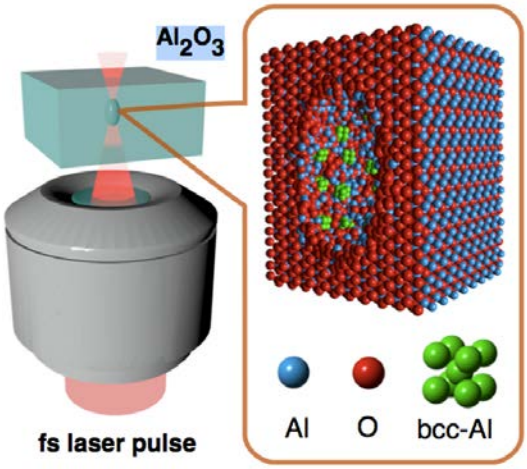


Figure 58. *An ultrafast (150 femtosecond) laser-induced micro-explosion is used to produce a super-dense, stable bbc-Al inside a sapphire slab.*

(**HPSynC**) and researchers from **Stanford**, **Australia National University**, **Zhizuoka University** and **Swinburne University of Technology** have now for the first time synthesized the bcc Al phase with an ultrafast, laser-induced confined micro-explosion inside a sapphire crystal and confirmed the new phase with high energy synchrotron XRD.

By focusing single short laser pulses of light onto a sapphire, it was possible to induce a micro-explosion to create locally ultrahigh pressure and temperature conditions inside the material (Fig. 58).[5]

3. EDUCATION, TRAINING, AND OUTREACH

In keeping with the goals of the SSAA program, the education and training of graduate students represents a top priority for CDAC, In addition, we support an extensive program of outreach to the broader high pressure community. This section describes the CDAC effort in this very important aspect of our Center.

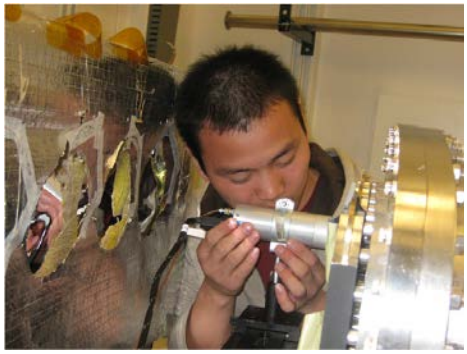


Figure 69. *CDAC graduate student* ***Jin Liu (UT Austin)*** *at the* ***APS****.*

3.1 CDAC Graduate Students and Post-doctoral Fellows

The main focus of the CDAC effort in its education, training and outreach mission is the support of graduate student preparation in the groups of the academic partners. CDAC graduate students carry out their dissertation research on a wide variety of problems in high *P-T* research relevant to stockpile stewardship, through projects in the fields of materials science, physics and chemistry as well as high-pressure mineral physics and geophysics (Figs. 59, 60). To date, 30 students have received the PhD degree with either full or partial support from CDAC.

The following graduate students in the research groups of CDAC Academic Partners received full or partial support of their graduate work through CDAC during 2011-2012.

Princeton (Duffy)	Jeffrey Finklestein
	Camelia Stan
Caltech (Fultz)	Lisa Mauger
	Jorge Munoz
	Sally Tracy
Berkeley (Wenk)	Waruntorn (Jane) Kanitpanyacharoen
	Pamela Kaercher
Alabama–Birmingham (Vohra)	Andrew Stemshorn
	Walter Uhoya
Illinois (Dlott)	Kathryn Brown
	Chris Berg
	Will Shaw
Arizona State (Yarger)	Samrat Amin
	Warner Weber
Yale (Lee)	Joseph O'Rourke (undergraduate)
	Yuejan Wang (postdoctoral)
	Kaveh Pahlevan (postdoctoral)
Florida International (Saxena)	Lyci George
	Rostislav Hrubiak
UCLA (Kavner)	Matt Armentrout
	Emma Rainey
Northwestern (Jacobsen)	Yun-yuan Chang
	Kimberly Adams
	Josh Townsend

Michigan (Li)	Jiachao Liu
Ohio State (Panero)	Daniel Reaman
	Jeffrey Pigott
Washington Univ. (Schilling)	Wenli Bi
	Jinhyuk Lim
Stanford (Mao)	Yu Lin
Texas-Austin (Lin)	Jin (Jeff) Liu
	Jing (Jill) Yang
	Nikki Seymour (undergraduate)
Michigan (Ewing)	Sul Gi Ye Park
	J. McLain Pray
Illinois (Cahill)	Greg Hohensee
	Wen-Pin Hsieh

The full list of graduate students who have received the PhD degree with CDAC support since the beginning of the program in 2003 is as follows:

James Patterson (Illinois, 2004)
Raja Chellappa (Nevada-Reno, 2004)
Wendy Mao (Chicago, 2005)
Jenny Pehl (Berkeley, 2005)
Tabitha Swan-Wood (Caltech, 2005)
Sergio Speziale (Princeton, 2006)
Alexander Papandrew (Caltech, 2006)
Nenad Velisavjevic (Alabama–Birmingham, 2006)
Emre Selvi (Texas Tech, 2007)
Joanna Dodd (Caltech, 2007)
Matthew Lucas (Caltech, 2008)
Resul Aksoy (Texas Tech, 2008)
Lowell Miyagi (Berkeley, 2009)
Chris Seagle (Chicago, 2009)
Bin Chen (Illinois, 2009)
Zhu Mao (Princeton, 2009)
Lyci George (Florida International, 2010)
Michael Winterrose (Caltech, 2010)
Erin Oelker (Arizona State, 2010)
Arianna Gleason (Berkeley, 2010)
Yahya Al-Khatatbeh (New Mexico State, 2010)
Susannah Dorfman (Princeton, 2011)
Xinyang Chen (Michigan, 2011)
Daniel Reaman (Ohio State, 2011)
Wenli Bi (Washington University, 2011)
Jeffrey Carter (Illinois, 2011)
Kathryn Brown (Illinois, 2012)
Wen-Pin Hsieh (Illinois, 2012)
Samrat Amin (Arizona State, 2012)
Rostislav Hrubiak (Florida International, 2012)

Figure 60. *CDAC partner* ***Kanani Lee (Yale)*** *and former CDAC graduate student* ***Yahya Al-Khatatbeh (New Mexico State)*** *at the* ***APS.***

Publications and presentations involving CDAC-supported students and postdoctoral fellows during 2011-2012 are as follows:

Student Publications

Adams, K. A., S. D. Jacobsen, Z. Liu, S. M. Thomas, M. Somayazulu, and D. M. Jurdy, Optical reflectivity of solid and liquid methane: Application to spectroscopy of Titan's hydrocarbon lakes, *Geophys. Res. Lett.* **39**, L04309 (2012).

Amin, S., E. N. Rissi, K. McKiernan, and J. L. Yarger, Determining the equation of state of amorphous solids at high pressure using optical microscopy, *Rev. Sci. Instrum.* **83**, 033702 (2012).

Amin, S. A., K. Leinenweber, C. J. Benmore, R. Weber, and J. L. Yarger, Characterizing pressure induced coordination changes in $CaAl_2O_4$ glass using ^{27}Al NMR, *J. Phys. Chem. C* **116**, 2068-2073 (2012).

Armentrout, M. M. and A. Kavner, High pressure, high temperature equation of state for Fe_2SiO_4 ringwoodite and implications for the Earth's transition zone, *Geophys. Res. Lett.* **38**, L08309 (2011).

Baldini, M., Y. Ding, S. Wang, Y. Lin, C. A. Tulk, A. M. Dos Santos, J. F. Mitchell, D. Haskel, and W. L. Mao, Pressure-induced tuning of a magnetic phase separation in $Nd_{0.53}Sr_{0.47}MnO_3$, *Phys. Rev. B* **86**, 094407 (2012).

Banks, H. B., W. Bi, L. Sun, G. F. Chen, X. H. Chen, and J. S. Schilling, Dependence of magnetic ordering temperature of doped and undoped $EuFe_2As_2$ on hydrostatic pressure to 0.8 GPa, *Physica C* **471**, 476 (2011).

Benmore, C. J., E. Soignard, M. Guthrie, S. A. Amin, J. K. R. Weber, K. McKiernan, M. C. Wilding, and J. L. Yarger, High pressure x-ray diffraction measurements on Mg_2SiO_4 glass, *J. Non-Cryst. Solids* **357**, 2632-2636 (2011).

Berg, C., A. Lagutchev, Y. Fu, and D. D. Dlott, Nitro stretch probing of a single molecular layer to monitor shock compression with picosecond time resolution, *AIP Conf. Proc.* **1426**, 1573 (2012).

Berg, C. M., K. E. Brown, R. W. Conner, Y. Fu, H. Fujiwara, A.Lagutchev, W. L. Shaw, X. Zheng, and D. D. Dlott, Experiments Probing Fundamental Mechanisms of Energetic Material Initiation and Ignition, *MRS Online Proceedings Library*, 1405 (2012).

Bi, W., Y. Meng, R. S. Kumar, A. L. Cornelius, W. W. Tipton, R. G. Hennig, Y. Zhang, C. Chen, and J. S. Schilling, Pressure-induced structure transition in europium metal to 92 GPa, *Phys. Rev. B* **83**, 104106 (2011).

Bi, W., N. M. Souza-Neto, D. Haskel, G. Fabbris, E. E. Alp, J. Zhao, R. G. Hennig, M. M. Abd-Elmeguid, Y. Meng, R. W. McCallum, K. Dennis, and J. S. Schilling, Synchrotron x-ray spectroscopy studies of valence and magnetic state in europium metal to extreme pressures, *Phys. Rev. B* **85**, 205134 (2012).

Brown, K. E., New technologies for spectroscopy of materials under static and shock compression, *Ph.D. Thesis, University of Illinois at Urbana-Champaign* (2012).

Brown, K. E., R. Conner, Y. Fu, and H. Fujiwara, Microscopic states of shocked polymers, *AIP Conf. Proc.* **1426**, 1593 (2012).

Brown, K. E., Y. Fu, W. L. Shaw, and D. D. Dlott, Time-resolved emission of dye probes in a shock-compressed polymer: Effects of te nanostructured energy landscape, *J. Appl. Phys.* **112**, 103508 (2012).

Brown, K. E., W. L. Shaw, X. Zheng, and D. D. Dlott, Simplified laser-driven flyer plates for shock compression science, *Rev. Sci. Instrum.* **83**, 103901 (2012).

Chen, B., W. P. Hsieh, D. G. Cahill, D. R. Trinkle, and J. Li, Thermal conductivity of compressed H_2O to 22 GPa: A test of the Leibfried-Sclömann equation, *Phys. Rev. B* **83**, 132301 (2011).

Chen, B., K. Lutker, S. V. Raju, J. Yan, J. Kanitpanyacharoen, J. Lei, S. Yang, H. R. Wenk, H. K. Mao, and Q. Williams, Pressure-promoted texturing in nanocrystalline nickle: Probing the lower size limit of dislocation activity, *Science* **338**, 1448-1451 (2012).

Chen, X. J., F. J. Jia, J. B. Zhang, Z. X. Qin, L. Y. Tang, L. J. Li, Z. A. Xu, J. Liu, V. V. Struzhkin, R. E. Cohen, and H. K. Mao, Pressure tuning of Fermi surface topology of optimally doped $BaFe_{1.9}Ni_{0.1}As_2$, *Phys. Rev. B*, submitted.

Duzynska, A., R. Hrubiak, V. Drozd, H. Teisseyre, W. Paszkowicz, A. Reszka, A. Kaminska, A. Durygin, S. K. Saxena, J. D. Fidelus, J. Grabis, C. J. Monty, and A. Suchocki, The structural and optical properties of ZnO bulk and nano crystals under high pressure *High Press. Res.*, in press.

Fu, Y., E. A. Friedman, K. E. Brown, and D. D. Dlott, Vibrational spectroscopy of nitroaromatic self-assembled monolayers under extreme conditions, *Chem. Phys. Lett.* **501**, 369-374 (2011).

Fujiwara, H., K. E. Brown, and D. D. Dlott, A thin-film Hugoniot measurement using a laser-driven flyer plate, *AIP Conf. Proc.* **1426**, 382 (2012).

George, L. and S. K. Saxena, Structural stability of metal hydrides, alanates and borohydrides of alkali and alkali- earth elements: A review, *Int. J. Hydrogen Energ.* **35**, 5454-5470 (2011).

Hrubiak, R., V. Drozd, A. Karbasi, and S. K. Saxena, High P-T phase transitions and P-V-T equation of state of hafnium, *J. Appl. Phys.* **111**, 112612 (2012).

Hsieh, W. P., M. D. Losego, P. V. Braun, S. Shenogin, P. Keblinski, and D. Cahill, Testing the minimum thermal conductivity model for amorphous polymers using high pressures, *Phys. Rev. B* **83**, 174205 (2011).

Kaercher, P., S. Speziale, L. Miyagi, W. Kanitpanyacharoen, and H. R. Wenk, Crystallographic preferred orientation in wustite (FeO) through the cubic-to-rhombohedral phase transition, *Phys. Chem. Minerals* **39**, 613-626 (2012).

Kanitpanyacharoen, W., S. Merkel, L. Miyagi, P. Kaercher, C. N. Tome, Y. Wang, and H. R. Wenk, Significance of mechanical twinning in hexagonal metals at high pressure, *Acta Mater.* **60**, 430-442 (2012).

Karbasi, A., S. K. Saxena, and R. Hrubiak, The thermodynamics of several elements at high pressure, *CALPHAD* **35**, 72-81 (2011).

Kavner, A., M. M. Armentrout, E. S. G. Rainey, M. Xie, B. E. Weaver, S. H. Tolbert, and R. B. Kaner, Thermoelastic properties of ReB_2 at high pressures and temperatures and comparison with Pt, Os, and Re, *J. Appl. Phys.* **110**, 093518 (2011).

Lin, J. F., J. Liu, C. Jacobs, and V. B. Prakapenka, Vibrational and elastic properties of ferromagnesite across the electronic spin-pairing transition of iron, *Am. Mineral.* **97**, 583-591 (2012).

Lin, Y., H. Ma, C. W. Matthews, B. Kolb, S. Sinogeiken, T. Thonhauser, and W. L. Mao, Experimental and theoretical studies on a high pressure monoclinic phase of ammonia borane, *J. Phys. Chem C* **16**, 2172-2178 (2012).

Lin, Y., Y. Yang, H. Ma, Y. Cui, and W. L. Mao, Compressional behavior of bulk and nanorod $LiMn_2O_4$ under nonhydrostatic stress, *J. Phys. Chem. C* **115**, 9844-9849 (2011).

Lin, Y., L. Zhang, H. K. Mao, P. Chow, Y. Xiao, M. Baldini, J. Shu, and W. L. Mao, Amorphous diamond - A high-pressure superhard carbon allotrope, *Phys. Rev. Lett.* **107**, 175504 (2011).

Lucas, M. S., L. Mauger, J. A. Munoz, Y. Xiao, A. O. Sheets, S. L. Semiatin, J. Horwath, and Z. Turgut, Magnetic and vibrational properties of high-entropy alloys, *J. Appl. Phys.* **109**, 07E307 (2011).

Mao, Z., J. F. Lin, S. D. Jacobsen, T. S. Duffy, Y. Y. Chang, J. R. Smyth, D. J. Frost, E. H. Hauri, and V. B. Prakapenka, Sound velocities of hydrous ringwoodite to 16 GPa and 673 K, *Earth Planet. Sci. Lett.* **331-332**, 112-119 (2012).

Mao, Z., J. F. Lin, J. Liu, A. Alatas, L. Gao, J. Zhao, and H. K. Mao, Sound velocities of Fe and Fe-Si alloys in the Earth's core, *Proc. Nat. Acad. Sci.* **109**, 10239-10244 (2012).

Mao, Z., J. F. Lin, J. Liu, and V. B. Prakapenka, Thermal equation of state of lower-mantle ferropericlase across the spin crossover, *Geophys. Res. Lett.* **38**, 23 (2011).

Miyagi, L., W. Kanitpanyacharoen, J. Knight, V. Raju, P. Kaercher, H. R. Wenk, Q. Williams, and E. Zepeda, Combined resistive and laser heating in diamond anvil high pressure experiments, *Rev. Sci. Instrum.*, submitted.

Miyagi, L., W. Kanitpanyacharoen, S. Stackhouse, B. Militzer, and H. R. Wenk, The effect of grain size on Deformation and texture development in $MgGeO_3$ post-perovskite, *Earth Planet. Sci. Lett.*, submitted.

Miyagi, L., W. Kanitpanyacharoen, S. Stackhouse, B. Militzer, and H. R. Wenk, The enigma of post-perovskite anisotropy: Deformation versus transformation textures, *Phys. Chem. Minerals* **38**, 665-678 (2011).

Munoz, J. A., M. S. Lucas, O. Delaire, M. Winterrose, L. Mauger, C. W. Li, A. O. Sheets, M. B. Stone, D. L. Abernathy, Y. Xiao, P. Chow, and B. Fultz, Positive vibrational entropy of chemical ordering in FeV, *Phys. Rev. Lett.* **107**, 115501 (2011).

Niu, H., X. Q. Chen, S. Wang, D. Li, W. L. Mao, and Y. Li, Families of superhard crystalline carbon allotropes constructed via cold compression of graphite and nanotubes, *Phys. Rev. Lett.* **108**, 135501 (2012).

Panero, W. R., J. R. Smyth, J. S. Pigott, Z. Liu, and D. J. Frost, Hydrous ringwoodite to 5 K and 35 GPa: Multiple hydrogen bonding sites resolved with FTIR spectroscopy, *Am. Mineral.*, in press.

Pigott, J. S., D. M. Reaman, and W. R. Panero, Microfabrication of controlled-geometry samples for the laser-heated diamond-anvil cell using focused ion beam technology, *Rev. Sci. Instrum.* **82**, 115106 (2011).

Reaman, D. M., Equation of state, diffusivity and deformation in the Fe-Ni alloy system to determine the structure and dynamics of Earth's inner core, *Ph.D. Thesis, Ohio State University* (2011).

Reaman, D. M., H. O. Colijn, F. Yang, and W. R. Panero, Interdiffusion of Earth's core materials to 65 GPa and 2200 K, *Earth Planet. Sci. Lett.* **349-350**, 8-14 (2012).

Reaman, D. M., G. S. Deahn, and W. R. Panero, Predictive mechanism for anisotropy development in the Earth's inner core, *Earth Planet. Sci. Lett.* **321**, 437-442 (2011).

Skinner, L. B., C. J. Benmore, S. Antao, E. Soignard, S. Amin, E. Bychkov, E. N. Rissi, J. B. Parise, and J. L. Yarger, Structural changes in vitreous $GeSe_4$ under pressure, *J. Phys. Chem. C* **116**, 2212-2217 (2012).

Stemshorn, A. K. and Y. K. VOhra, Compression of bulk metallic glass $Zr_{57}Cu_{15.4}Ni_{12.6}Al_{10}Nb_5$, *Am. Mineral.* **31**, 287-291 (2011).

Tsoi, G., W. Malone, W. Uhoya, J. E. Mitchell, Y. K. Vohra, L. E. Wegner, A. S. Sefat, and S. T. Weir, Pressure induced superconductiviyt in $Ba_{0.5}Sr_{0.5}Fe_2As_2$, *J. Phys.: Cond. Matt.* **24**, 495702 (2012).

Uhoya, W., J. M. Montgomery, G. K. Samudrala, G. Tsoi, Y. Vohra, S. T. Weir, and A. S. Sefat, High-pressure structural phase transitions in chromium-doped $BaFe_2As_2$, *J. Phys.: Conf. Series* **337**, 012016 (2012).

Uhoya, W., G. Tsoi, Y. Vohra, N. Wolanyk, S. M. Rao, M. K. Wu, and S. T. Weir, Simultaneous measurement of pressure evolution of crystal structure and superconductivity in $FeSe_{0.92}$ using designer diamonds, *Europhys. Lett.* **99**, 26002 (2012).

Uhoya, W. O., J. M. Montgomery, G. M. Tsoi, Y. K. Vohra, M. A. McGuire, A. S. Sefat, B. C. Sales, and S. T. Weir, Phase transition and superconductivity of $SrFe_2As_2$ under high pressure, *J. Phys.: Cond. Matt.* **23**, 122201 (2011).

Uhoya, W. O., G. M. Tsoi, Y. K. Vohra, and A. S. Sefat, Structural phase transitions in EuFe2As2 superconductor at low temperatures and high pressures, *J. Phys.: Cond. Matt.* **23**, 365703 (2011).

Wang, J., W. Yang, S. Wang, X. Xiao, F. De Carlo, Y. Liu, and W. L. Mao, High pressure nano-tomography using an iterative method, *J. Appl. Phys.* **111**, 112626 (2012).

Wang, S., Y. F. Meng, N. Ando, M. Tate, S. Krasnicki, C. S. Yan, Q. Liang, J. Lai, H. K. Mao, S. M. Gruner, and R. J. Hemley, Single-crystal CVD diamonds as small-angle x-ray scattering windows for high pressure research, *J. Appl. Cryst.* **45**, 453-457 (2012).

Wang, S., X. Yu, Z. Lin, R. Zhang, D. He, J. Qin, J. Zhu, J. Han, L. Wang, H. K. Mao, J. Zhang, and Y. Zhao, Synthesis, crystal structure, and elastic properties of novel tungsten nitrides, *Chem. Mater.* **24**, 3023-3028 (2012).

Winterrose, M. L., L. Mauger, I. Halevy, A. F. Yue, M. S. Lucas, J. A. Munoz, H. Tan, Y. Xiao, P. Chow, W. Sturhahn, T. S. Toellner, E. E. Alp, and B. Fultz, Dynamics of Fe atoms across the pressure-induced Invar transition in Pd_3Fe, *Phys. Rev. B* **83**, 134304 (2011).

Xie, M., R. Mohammadi, Z. Mao, M. M. Armentrout, A. Kavner, R. B. Kaner, and S. H. Tolbert, Exploring the high-pressure behavior of superhard tungsten tetraboride, *Phys. Rev. B* **85**, 064118 (2012).

Ye, Y., D. A. Brown, J. R. Smyth, W. R. Panero, S. D. Jacobsen, Y. Y. Chang, J. P. Townsend, S. M. Thomas, E. H. Hauri, P. Dera, and D. J. Frost, Compressibility and thermal expansion of hydrous ringwoodite with 2.5(3) wt% H_2O, *Am. Mineral.* **97**, 573-582 (2012).

Student Presentations

Adams, K., S. D. Jacobsen, Z. Liu, M. Somayazulu, S. M. Thomas, and D. M. Jurdy, Visible and near-infrared reflectivity of solid and liquid methane: application to spectroscopy of Titan's hydrocarbon lakes, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Adams, K. A., S. D. Jacobsen, S. M. Thomas, Z. Liu, M. Somayazulu, and D. M. Jurdy, Visible and infrared reflectivity of solid and liquid methane: Application to hydrocarbon lakes on Titan, *42nd Lunar and Planetary Science Conference* (The Woodlands, TX, March 7-11, 2011).

Armentrout, M., Fiber reinforced composites under pressures: A case study in non-hydrostatic behavior in the diamond anvil cell, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Armentrout, M. A. and A. Kavner, Comparative thermal equations of state for transition metal (Fe, Ni, Co) ringwoodites and implications for the Earth's chemical evolution, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Armentrout, M. M. and A. Kavner, Comparative thermoelastic properties of FeO, NiO, and CoO at high pressures and temperatures: Implications for element partitioning in the mantle, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Berg, C., Laser-driven shock compression of an explosive simulant monolayer, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Berg, C., Picosecnd time-resolved shock complression of energetic materials, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Berg, C. M., Nitro stretch probing of a single molecular layer to monitor shock compression with picosecond time resolution, *17th APS SCCM Conference* (Chicago, IL, July, 2011).

Bi, W., Pressure-induced structure transitions in europium metal to 92 GPa, *APS March Meeting* (Dallas, TX, March 21-25, 2011).

Bi, W., High-pressure studies of valence and magnetic state in europium metal, *APS March Meeting* (Dallas, TX, March 21-25, 2011).

Bi, W., Magnetism and superconductivity under extreme pressure in rare earth elements (invited), *Advanced Photon Source, Argonne National Laboratory* (Argonne, IL, February 9, 2011).

Bi, W., High-Pressure Studies of Structure, Valence, and Magnetism in Europium Metal to 92 GPa, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Bi, W., G. Fabbris, J. Schilling, N. Souza-Neto, D. Haskel, J. Zhao, E. E. Alp, Y. Meng, and A. Alsmadi, High-pressure studies of valance and magnetic state in europium metal, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Bi, W., J. Schilling, Y. Meng, R. Kumar, A. Cornelius, Y. Zhang, C. Chen, and R. Hennig, Pressure-induced structure transition in europium metal to 92 GPa, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Bishop, M., W. Uhoya, G. Tsoi, Y. K. Vohra, A. Sefat, and B. C. Sales, Formation of collapsed tetragonal phase in $EuCo_2As_2$, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Brown, K., Emission spectroscopy of shocked materials, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).
Brown, K., Time-resolved emission spectroscopy of shocked materials, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).
Brown, K. E., Static and shock compression of materials, *Los Alamos National Laboratory* (Los Alamos, NM, December, 2011).
Brown, K. E., Microstates of a shocked polymer, *Shock Compression of Condensed Matter* (June, 2011).
Brown, K. E. and W. Shaw, Optimizing laser-driven flyer plates for studying time-resolved emission of shocked materials, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).
Chang, Y. Y., Electronic spin transition of iron in dense hydrous magnesium silicate at high pressure, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).
Chang, Y. Y., Electronic spin transition of iron in dense hydrous magnesium silicate at high pressure, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).
Chang, Y. Y., S. D. Jacobsen, J. F. Lin, J. Wu, D. J. Frost, S. M. Thomas, P. K. Dera, Y. Xiao, P. Chow, and G. Shen, Electronic spin transition of iron in dense hydrous magnesium silicate phase D at high pressure, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Chen, B., D. Zhang, W. Leng, J. M. Jackson, Y. Wang, T. Yu, J. Liu, and J. Li, Rapid terrestrial core formation from *in situ* x-ray computed microtomography (invited), *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Dalton, D. A., A. F. Goncharov, W. P. Hsieh, and D. Cahill, High P-T thermal conductivity of periclase using an ultrafast pump-probe method, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Duffy, T. S. and C. V. Stan, Elastic properties of mantle minerals (invited), *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Farfan, G., S. Wang, and W. L. Mao, Raman study of opal at high pressure, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Farfan, G. A., S. Wang, E. Boulard, and W. L. Mao, High pressure behavior of 3d transition metal carbonates, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Finkelstein, G., New insights into high-pressure materials from synchrotron-based single-crystal x-ray diffraction, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).
Finkelstein, G. J., P. K. Dera, and T. S. Duffy, Single-crystal x-ray diffraction of pyrope garnet to 84 GPa, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Finkelstein, G. J., P. K. Dera, C. M. Holl, Y. Meng, and T. S. Duffy, Single-crystal x-raey diffraction of foresterite to 90 GPa, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Finkelstein, G. J., P. K. Dera, Y. Meng, and T. S. Duffy, New insights into the high-pressure behavior of olivine from single-crystal x-ray diffraction (invited), *Single Crystal Diffraction under Extreme Conditions Workshop, Advanced Light Source User's Meeting*, 2011).
Fu, Y., E. Friedman, K. Brown, and D. Dlott, High pressure vibrational spectroscopy of molecular monolayers, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).
Hernlund, J. W., K. Ohta, H. Gomi, E. S. Rainey, K. Hirose, S. Labrosse, R. Caracas, A. Kavner, L. Pilon, and C. T. Houser, Preliminary core-mantle boundary heat flux map (invited), *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Hohensee, G., High pressure thermal conductivity measurements of amorphous, crystalline, and alloy materials, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).
Hou, Y., Y. Lin, and W. L. Mao, X-ray diffraction and Raman spectroscopy study of pressure induced transition in [1,2,3]tetramantane, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Hrubiak, R., Thermal conductivity of zirconium at high pressure and temperture in a laser heated DAC, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).
Hrubiak, R., Measuring thermal conductivity of materials under high temperatures and pressures in a laser heated diamond anvil cell, *Advanced School on the New Developments in Field of Snchrotron Radiation* (Brazilian Synchrotron Light Laboratory, Campinas, SP, Brazil, February, 2011).
Hrubiak, R., High-pressure x-ray diffraction study of $SrVO_3$ and $CaVO_3$ perovskite oxides, *SMEC 2011 Meeting* (Belize and Mexico, April-March, 2011).
Hrubiak, R., Thermal conductivity of zirconium at high pressure and temperature in a laser heated DAC, *SMEC 2011 Meeting* (Belize and Mexico, April-March, 2011).

Hrubiak, R., High P-T phases and P-V-T equation of state of hafnium, *SMEC 2011 Meeting* (Belize and Mexico, April-March, 2011).

Hrubiak, R., High P-T structure and P-V-T equation of state of hafnium, *Consortium for Materials Properties Research in Earth Sciences (COMPRES) Annual Meeting* (Williamsburg, VA, June 2011).

Hrubiak, R., Equations of state of group IVB transition metals (Ti, Zr, Hf) at high temperatures and pressures, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Hsieh, W. P., Development of metal film transducers for time-domain thermoreflectance at high pressures, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Hsieh, W. P., M. Losego, P. Braun, S. Shenogin, P. Keblinski, and D. Cahill, Testing the minimum thermal conductivity model for amorphous polymers under high pressure, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Hsieh, W. P., A. Lyons, E. Pop, P. Keblinski, and D. Cahill, Pressure tuning of the thermal conductance of weak interfaces, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Kaercher, P., Crystallographic preferred orientation in FeO through the cubic-to-rhombohedral phase transition, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Kaercher, P., Texture of FeO during phase transition, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Kaercher, P., Two-phase deformation of lower mantle mineral analogs, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Kaercher, P. M., B. Militzer, and H. R. Wenk, Ab initio calculations of elastic constants of plagioclase feldspar, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Kaercher, P. M., S. Speziale, L. M. Miyagi, W. Kanitpanyacharoen, and H. R. Wenk, Texture development in FeO across the cubic to rhombohedral phase transition, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Kanitpanyacharoen, J., *In situ* laser and resistive heating techniques of Fe and (Mg,Fe)O at high pressure in radial diffraction geometry, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Kanitpanyacharoen, W., *In situ* laser and resistive heating techniques at high pressure in radial diffraction geometry, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, february 15-17, 2011).

Kanitpanyacharoen, W., Preferred orientation and phase transformation of zirconium under high pressure and temperature, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Kanitpanyacharoen, W., D. Dewhurst, M. Raven, and H. R. Wenk, Texture and anisotropy of shales from the Officer Basin, Western Australia, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Kanitpanyacharoen, W., H. R. Wenk, S. Matthies, and R. Vasin, Self-containing modeling of elastic anisotropy in shale, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Kavner, A. and M. A. Armentrout, High-pressure high-temperature equation of state of B1 cobalt oxide and implications for redox relations in the Earth's lower mantle, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Lim, J., Studies of magnetism and superconductivity under extreme pressure, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Lin, J. F., Z. Mao, C. Lu, S. D. Jacobsen, T. S. Duffy, Y. Y. Chang, D. J. Frost, E. H. Hauri, K. K. Zhuravlev, S. N. Tkachev, and V. Prakapenka, Sound velocities of the transition zone minerals (invited), *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Lin, Y., L. Zhang, H. K. Mao, P. Chow, Y. Xiao, M. Baldini, J. Shu, and W. Mao, Amorphous diamond - A high-pressure superhard carbon allotrope, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Liu, J., Elasticity of iron alloys in Earth's inner core, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Liu, J., Tandem magnetic transition in compressed Fe_7C_3, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Liu, J., J. F. Lin, Z. Mao, A. Alatas, L. Gao, J. Zhao, and L. S. Dubrovinsky, Compressional wave velocity of Fe alloys in Earth's core, *COMPRES Annual Meeting* (Williamsburg, VA, June, 2011).

Liu, J. and C. Lu, Sound velocity of iron and iron alloy measured at by high-energy resolution inelastic x-ray scattering (HERIXS), *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Liu, J., B. O. Mysen, Y. Fei, H. K. Mao, R. J. Hemley, and J. Li, Temperature dependent Mossbauer spectra of aluminous perovskite and implications for the Earth's lower mantle, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Mao, W. L., Y. Lin, W. Yang, and J. Wang, Nanoscale x-ray imaging of deep carbon (invited), *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Mao, Z., J. F. Lin, S. D. Jacobsen, T. S. Duffy, Y. Y. Chang, D. J. Frost, E. H. Hauri, and V. Prakapenka, Elasticity of hydrous ringwoodite in Earth's transition zone, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Mauger, L., Anharmonic behavior in Fe near the α-γ structure phase transition, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Mauger, L., Anharmonic behavior in Fe near the α-γ structural phase transition, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Mauger, L., M. Kresch, M. Lucas, J. Munoz, Y. Xiao, and B. Fultz, Anharmonic phonon behavior in □-Fe at temperatures near the structural phase transition, *TMS Annual Meeting - Approaches for Investigating Phase Transformations at the Atomic Scale* (San Dieg, CA, March 2, 2011).

Mauger, Y., Polaron hopping in $LiFePO_4$ at elevated pressures and temperatures, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

McKiernan, K. and S. Amin, High-pressure Brillouin spectroscopy of basaltic glasses and characterizing pressure induced structural changes in glasses and liquids using NMR, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Munoz, J., Large softening of the phonon partial densities of states of C15 rare-earth-iron compounds, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Munoz, J., Phonon density of states and high pressure thermodynamics of MgB_2, *TMS Annual Meeting - Brent Fultz Honorary Symposium* (San Diego, CA, February 28, 2011).

Munoz, J., Positive vibration entropy of chemical ordering in FeV, *2011 Joint Annual Conference of the National Society of Black Physicists and the National Society of Hispanic Physicists* (Austin, TX, September, 2011).

Munoz, J., Large softening of the phonon partial densities of states of C15 rare-earth-iron compounds, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Panero, W. R., J. R. Smyth, D. M. Reaman, J. S. Pigott, C. T. Unterborn, D. J. Frost, and Z. Liu, The effects of iron and water on elastic properties of ringwoodite from theory and experiment: Constraint on chemical and thermal variations in the transition zone (invited), *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Pigott, J., Microfabrication of controlled-geometry samples for the laser-heated diamond-anvil cell using focused ion beam technology, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Pigott, J. S., D. Reaman, and W. R. Panero, Microfabrication of controlled-geometry samples for the laser-heated diamond-anvil cell using focused ion beam technology, *COMPRES Annual Meeting* (Williamsburg, VA, June, 2011).

Pigott, J. S., D. M. Reaman, and W. R. Panero, Microfabrication of controlled-geometry samples for the laser-heated diamond-anvil cell using focused ion beam technology, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Pray, J. M., Behavior of actinide-bearing materials under extreme conditions, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Queen, D., J. Karel, X. Liu, G. Hohensee, D. Cahill, and F. Hellman, Two level systems in amorphous silicon, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Rainey, E. S., A. Kavner, J. W. Hernlund, and L. Pilon, Measuring thermal conductivity at high pressure and temperature in the laser-heated diamond anvil cell, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Rainey, E. S., A. Kavner, J. W. Hernlund, L. Pilon, and M. Veitch, Heat flow in the laser-heated diamond anvil cell and the thermal conductivity of iron-bearing oxides and silicates at lower mantle pressures and temperatures, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Reaman, D., Viscosity constraints of Earth's inner core, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Reaman, D., H. O. Colijn, and W. R. Panero, High-pressure, high-temperature diffusion measurements in iron-nickle alloys to 65 GPa, *COMPRES Annual Meeting* (Williamsburg, VA, June, 2011).

Reaman, D. M., G. Daehn, and W. R. Paneron, Inner-core anistotropy: Bridging our understanding between seismology and mineral physics (invited), *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Reaman, D. M., W. R. Panero, and H. Colijn, High-pressure, high-temperature diffusion measurements in iron-nickel alloys to 65 GPa, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Sorini, A. P., C. C. Chen, S. Wang, W. L. Mao, T. P. Devereaux, and C. C. Kao, Theoretical x-ray spectroscopy for strongly correlated materials at high pressure, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Stan, C. V., V. Prakapenka, and T. S. Duffy, Post-cotunnite phases in the AX2 system: Compression of PbF_2 to 80 GPa, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Thomas, S., W. Uhoya, L. Wegner, and Y. K. Vohra, Magnetic phase transition in rare earth metal holmium at low temperatures and high pressures, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Townsend, J., Mbar-presesure synchrotron-IR of laser-heated materials in the diamond anvil cell, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Townsend, J. C., Y. Y., X. Lou, S. Kirklin, J. Doak, A. Issa, S. Tkachev, P. K. Dera, and S. D. Jacobsen, Stability of post-aragonite $BaCO_3$ to 130 GPa and 2000 K, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Uhoya, W., Anomalous compressibility effects and superconductivity in 1-2-2 iron-base superconductors under high pressure, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Uhoya, W., Collapsed tetragonal phae and superconductivity in 112 compounds, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Uhoya, W., Simultaneous measurement of pressure evolution of crystal structure and superconductivity in $FeSe_{0.92}$ using designer diamonds, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Uhoya, W., N. Wolanyk, G. Tsoi, Y. K. Vohra, S. M. Rao, M. K. Wu, and S. T. Weir, Simultaneous measurement of pressure evolution of crystal structure and superconductivity in $FeSe_{0.8}$ using designer diamonds, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Wang, S., High pressure chemistry of SiH_4 and H_2O, *American Chemical Society National Meeting* (Denver, CO, August, 2011).

Wang, S., S. Hirai, A. Kemper, M. Baldini, H. Ma, S. Riggs, M. Shapiro, T. Devereaux, I. Fisher, W. Mao, and T. Geballe, High pressure study of mixed valence comound $CsAuI_3$, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Winterrose, M. L., L. Mauger, J. Munoz, and B. Fultz, Pressure induced invar anomaly in Pd_3Fe, *The 6th Annual Nassau-Argonne International Mossbauer Symposium* (Garden City, NJ, January 13, 2011).

Yamanaka, T., A. Kyono, S. Kharlamova, E. Alp, W. Bi, and H. K. Mao, Electron spin transition causing structure transformations of earth's interiors under high pressure, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Yang, F., Y. Lin, and W. L. Mao, Diamondoids under high pressure, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Yang, J., Vibrational and elastic properties of ferromagnesite across the electronic spin pairing tansition of iron, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Zepeda-Alarcon, E., J. W. Knight, A. MacDowell, L. M. Miyagi, P. M. Kaercher, W. Kanitpanyacharoen, H. R. Wenk, and Q. C. Williams, Resistive heating in radial geometry diamond anvil cell, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

3.2 Undergraduate Student Summer Scholars

A number of university undergraduate students participating in the highly successful Carnegie Summer Scholars Program have worked in the high pressure group at Carnegie, and have carried out research with CDAC personnel. The Summer Scholars Program, which is run by CDAC coordinator **Stephen Gramsch**, seeks to identify promising students who may not have had the opportunity to engage in research during the academic year. At **Carnegie**, such students experience a rigorous introduction to scientific research, and through the

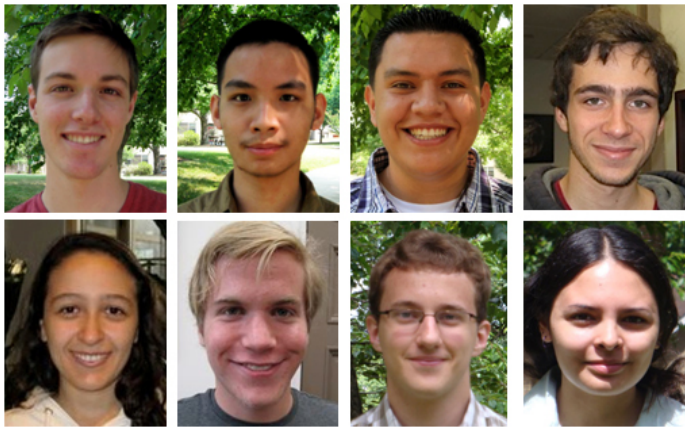


Figure 61. *Top, Ari Benjamin, Tao Liu, Kevin Hernandez, Louis Loubeyre. Bottom: Juliana Mesa, Maimon Rose, Viktor Rosza, Nichole Valdez.*

CDAC group meeting setting, are learning about the important problems in the field of high-pressure research. During the summers of 2011-2012, the following students worked with the Carnegie group (Fig. 61).

Students funded by CDAC are designated with an asterisk in the list below (*).

2011:

Ari Benjamin*, Williams College
EOS of the Fluorinated Copolymer Kel-F 800 to Near Megabar Pressures
Kevin Hernandez*, California State University – Sacramento
Raman Spectroscopy Studies of the Carbon Dioxide-Water System at High Pressure
Tao Liu, Howard County Community College
Optical Emission Spectroscopy Studies of MPCVD Diamond Growth

2012:

Louis Loubeyre, University of Paris VII
Heterogeneity in the Dynamics of Methanol under High Pressure
Juliana Mesa*, Universidad EAFIT, Columbia (US Citizen)
Geochemistry of Fe Stable Isotopes: From Planets to Minerals
Maimon Rose, University of Chicago
Investigating the Electrocaloric and Piezoelectric Effects in $LiNbO_3$ and PMN-PT using MD Simulations
Viktor Rozsa*, Hillsdale College
Pressure Studies of Hydrogen-Loaded Hydroquinone Clathrate
Nichole Valdez*, Colorado College
High Pressure Synthesis of Fe_2SiO_5

A group of participants from the National School on Neutron and X-Ray Scattering (NX School), which was held at the APS from August 12-25, 2012, attended the High Pressure Diffraction class at **HPCAT** from August 13-15 (Fig. 62). At beamline 16-BM-D, Beamline Scientists **Changyong Park** and **Dmitry Popov** gave an intensive set of lessons, complimented by hands-on experimentation and data analysis. Students learned about the basic mechanics of DACs, automated pressure control and monitoring systems, and on-line pressure measurement. In the hands-on portion of the course, students worked through an experiment on the hexagonal to cubic phase transition of ZnO at 10 GPa and room temperature.

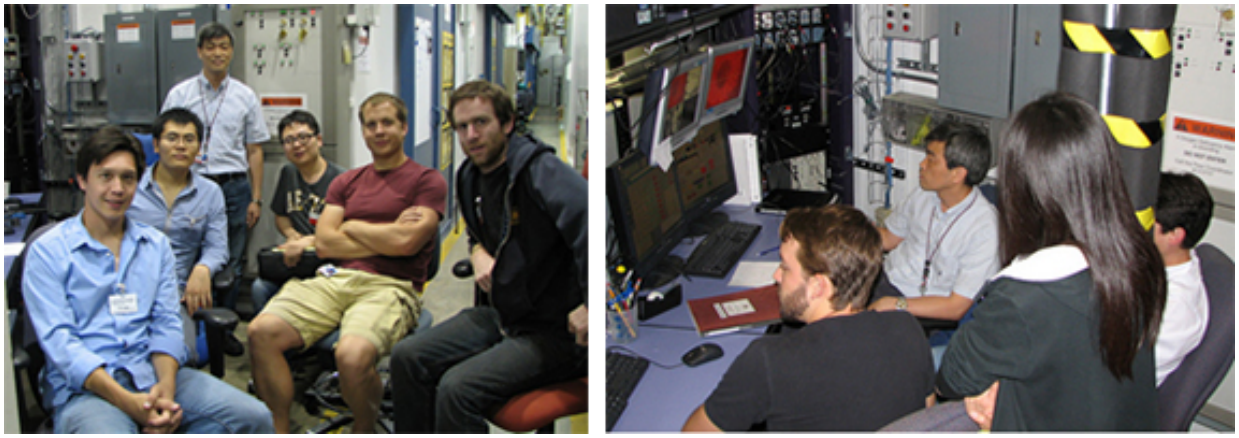


Figure 62 *Left: group of students from the NX school that participated in the HPCAT High Pressure Diffraction course. Right: Changyong Park demonstrates the alignment of a diamond cell sample in the x-ray beam at 16-BM-D.*

3.3 High School Outreach

Every year at **Carnegie**, one or two local high school students are hosted by CDAC and offered guidance in their science fair projects and in other areas of research.

2011:

Pei-Nan Chen, Poolesville High School, Poolesville, MD
Behavior of Methane Under High P-T Conditions using Raman and IR Spectroscopy

2012:

Thomas McHale, Montgomery Blair High School, Silver Spring, MD
Simulation of Electrocaloric Materials using Molecular Dynamics

2011 **Carnegie** High School intern **Pei-Nan Chen** (**Poolesville High School**) was been named a semifinalist in the 2012 Intel Science Talent Search (STS). Only 300 high school seniors around the country are selected out of more than 1,800 applicants to be semifinalists. Pei-Nan worked in the high-pressure labs at **Carnegie** with **Chang-sheng Zha** on the behavior of methane over a broad range of conditions of temperature and pressure using Raman and IR spectroscopy. His research has led to an identification of phase transitions of solid methane up to pressures of 43 GPa. He also has established an extended phase diagram of methane to pressures of 35 GPa and temperatures of 900 K. The results have implications for planetary science and the concentration of hydrocarbons in the Earth. Alumni of the STS have made extraordinary contributions to science and hold more than 100 of the world's most coveted science and math honors, including seven Nobel Prizes and four National Medals of Science. He also was the first author on a paper published in *Physical Review B*.[105]

***Figure 63** . Top, Students at 2012 Science Careers in Search of Women Conference at APS visit HPCAT. Bottom: Beamline Scientist Yue Meng demonstrates the use of pressure measurement instrumentation at 16-ID-B.*

2010 **Carnegie** High School intern **Winston Liu** (**Montgomery Blair High School**) was named a semifinalist in the Intel STS for 2011. His study, "Ethane-Hydrogen Systems under High Pressure," was conducted in the high-pressure labs under the direction of **Jinfu Shu** and **Ho-kwang Mao**.

At **UT-Austin**, the **Lin** group collaborated with the UTeach program to provide 4th-7th grade students participating in math- and science-focused summer camps with a tour of their laboratories. Students and undergraduates preparing for teaching careers in math and science learned about the crystal structure of a diamond and how the structure makes it especially useful in high-temperature high-pressure experiments, passed around a DAC, observed ruby fluorescence, and learned about the relationship between pressure and area and how it is exploited in the DAC. The students learned how Raman spectroscopy and the DAC can be used to study different phases of minerals and how this can be applied to determining the composition of the Earth's deep interior.

Upper level high school women from the Chicago area toured **HPCAT** on April 19, 2012 as part of the "Science Careers in Search of Women" Conference at ANL. **HPCAT** Beamline Associate

Genevieve Boman gave a presentation on high pressure science at **HPCAT**, and discussed her own science background and role as beamline associate. Beamline Scientist **Yue Meng** headed a tour at the 16-BM-D hutch, where CDAC Scientist **Maddury Somayazulu** (**Carnegie**) was conducting an experiment. He spoke with the girls about his experiment on single crystal diffraction of xenon compounds (Fig. 63).

3.4 CDAC Collaborators

CDAC also has established active collaborations with high-pressure groups throughout the country and around the world. These collaborations play an important role fulfilling the mission of the center, specifically by training new students and researchers in high-pressure materials science and exposing them to problems of importance to the NNSA Labs. Some other collaborations are just starting and still others that are in the preliminary planning stages, but in all cases the infrastructure made possible by CDAC has provided the leverage needed to work on a number of exciting new research directions. The CDAC collaborators from 2011-2012 include faculty and students from the following institutions:

Academia Sinica, Taiwan
S. M. Rao
M. K. Wu
Agency for Defense Development, Korea
K. J. Kim
Y. H. Ko
Airforce Research Laboratory
J. Horwath
M. Lucas
S. L. Semiatin
A. O. Sheets
Z. Turgut
Ames Laboratory
K. Dennis
R. W. McCallum
Amherst College
D. Ang
J. Gordon
L. Hunter
S. Peck
Argonne National Laboratory
A. Alatas
J. D. Almer
E. E. Alp
C. Benmore
W. Bi
Z. Cai
F. De Carlo
Y. Ding
G. Fabbris
L. Gao
R. Harder
D. Haskel
J. F. Mitchell
J. S. Okasinski
S. Peng
V. B. Prakapenka
J. Quintana
Y. Ren
B. Rusthoven
J. A. Schlueter
N. Souza-Neto

Argonne National Laboratory, cont'd
W. Sturhahn
Y. Sun
M. van Veendaal
S. Wang
Y. Wang
R. Weber
X. Xiao
J. Zhao
M. Zhernenkov
Arizona State University
K. Leinenweber
E. Soignard
Auburn University
J. Dong
M. Ntam
Austrailia National University
E. G. Gamaly
A. V. Rode
Australian Nuclear Science and Technology Organization
G. J. McIntyre
Bard College at Simons Rock
Y. Al-Khatatbeh
Beijing Computational Science Research Center
C. Zhang
Beijing Institute of Spacecraft Environment Engineering, China
Z. Gong
Beijing University of Technology, China
X. D. Han
Bhabha Atomic Research Centre, India
S. N. Achary
R. Shukla
A. K. Tyagi
Bharathidasan University, India
S. Arumugam
S. Esakki Muthu
M. Kanagaraj

Brookhaven National Laboratory
G. L. Carr
Z. Chen
W. Q. Han
California Institute of Technology
B, Chen
J. M. Jackson
C. W. Li
X. Tang
D. Zhang
Carnegie Institution of Washington
M. L. Fogel
P. L. Griffin
E. H. Hauri
A. Kish
K. L. Rogers
A. Steeele
CEA, France
I. Goncharenko
P. Loubeyre
F. Occelli
CERAMATEC Inc.
S. Balagopal
A. Nickens
China Academy of Engineering Physics
L. Cai
Chinese Academy of Sciences
L. Bai
G. Chen
X. Chen
X. Q. Chen
X. Dai
Z. Deng
X. Dong
Z. Fang
S. M. Feng
P. Gao
H. M. Gong
D. Gu
J. Guo
J. G. Guo
S. Jiang
C. Q. Jin
P. P. Kong
A. Li
D. Li
X. Li
Y. Li
C. Lin
H. Q. Lin
J. Liu
Q. Q. Liu
Y. Liu
Y. Lu
Y. Lv
H. Niu
L. Sun
L. Tang
X. Wang

Chinese Academy of Sciences, cont'd
X. C. Wang
H. M. Weng
G. F. Wu
Q. Wu
W. Xiao
H. Xie
K. Yang
L. Yang
L. X. Yang
R. C. Yu
R. Z. Yu
X. Yu
C. Zhang
J. L. Zhang
S. J. Zhang
W. Zhang
Y. Zhang
Z. Zhao
G. H. Zhong
J. Zhu
Cornell University
N. W. Ashcroft
S. M. Gruner
R. G. Henning
R. Hoffmann
V. Labet
M. Tate
W. W. Tipton
S. Wang
P. Zaleski-Ejgierd
Deutches Elektron-Synchrotron, Germany
H. P. Liermann
Duke University
J. Contreras-Garcia
Eastern Washington University
J. L. Manson
École Polytechnique Fédérale de Lausanne, Switzerland
H. Berger
Ehime University, Japan
T. Inoue
T. Irifune
A. Yamada
Eindhoven University of Technology, The Netherlands
H. T. Hintzen
European Synchrotron Radiation Facility, France
E. Borissenko
S. Evans
M. Hanfland
A. Kantor
I. Kantor
M. Mezouar
S. Pascarelli
A. C. Walters

Florida International University
J. Chen
V. Drozd
S. Garimella
L. George
A. Karbasi
Florida State University
H. D. Zhou
George Mason University
H. W. Sheng
Goethe-Universität Frankfurt, Germany
E. Haussühl
Hallym University, Korea
J. Y. Choi
M. S. Jeong
J. H. Kim
J. H. Ko
Hameshite University, Jordan
A. Alsmadi
Hangzhou Normal University, China
J. Dai
K. Yang
Harbin Institute of Technology, China
L. Z. Cao
L. Kong
H. Z. Liu
L. Wang
Harima Institute, Japan
A. Kotani
M. Taguchi
H. Yamaoka
Hebei University of Technology, China
C. L. Qin
High Energy Accelerator Research Organization, Japan
K. Ikeda
H. Ohshita
T. Otomo
High Performance Computing Center Stuttgart, Germany
C. W. Glass
Hiroshima University
M. Arita
K. Doi
T. Ichikawa
Y. Kojima
H. Namatame
K. Shimada
M. Taniguchi
M. Tsubota
Howard University
Y. Kandry
M. Mahmood
Hubei University
Z. B. Huang
Illinois Wesleyan University
N. Wolanyk
Imperial College London, UK
S. G. MacLeod
Indian Institute of Technology, India
A. K. Ganguli
J. Prakash
G. S. Thakur
Indiana University – South Bend
H. P. Scott
Indira Ghandi Centre for Atomic Research, India
T. Ravindran
V. Sivasubramanian
N. Subramanian
Institut Laue-Langevin, France
L. Capogna
Institute for Molecular Science, Japan
M. Matsunami
Japan Agency for Marine-Earth Science and Technology
K. N. Matsukage
Japan Atomic Energy Agency
K. Aoki
H. Arima
T. Hattori
M. Honda
I. Jarrige
Y. Katayama
A. Machida
A. Sano-Furukawa
K. Suzuya
T. Watanuki
Japan Synchrotron Radiation Institute
Y. Ikemoto
T. Moriwaki
H. Ohashi
Y. Ohishi
Y. Senba
Jilin University
T. Cui
D. Duan
X. Huang
X. Jin
B. Li
D. Li
Q. Li
S. Li
Z. Li
B. Liu
B. B. Liu
R. Liu
Y. Ma
Y. Sui
X. Tan
F. Tian
J. Wang
K. Wang
L. Wang
X. Wang
Y. Wang
Z. Wang
W. Wu
R. Xu

Jilin University, cont'd
T. Yan
Y. Yan
X. Yang
J. Yu
M. Zhang
X. Zhao
M. Zhou
L. Zhu
B. Zou
G. Zou
X. Zou
Johns Hopkins University
Y. Q. Cheng
E. Ma
M. Xu
Kobe University, Japan
M. Matsunami
I. Matsutori
K. Miyata
N. Ohta
H. Okamura
K. Shoji
H. Sugawara
A. Takigawa
Kongju National University, Korea
J. W. Lee
Korea Atomic Energy Research Institute
S. Y. Lee
Korea Maritime University
J. H. Yoon
KTH Royal Institute of Technology, Sweden
A. B. Belonoshko
Laboratorio Nacional de Luz Sincrotron, Brazil
N. M. Souza-Neto
Lawrence Berkeley National Laboratory
B. Chen
S. V. Raju
C. R. Rotundu
J. Yan
Lawrence Livermore National Laboratory
M. R. Armstrong
S. Bastea
K. J. M. Blobaum
J. A. Bradley
N. P. Butch
P. M. Celliers
J. Y. Chen
G. W. Collins
J. C. Crowhurst
H. Cynn
J. H. Eggert
W. J. Evans
D. Fujino
D. G. Hicks
W. M. Howard
J. H. Klepeis
J. R. Jeffries
Z. Jenei

Lawrence Livermore National Laboratory, cont'd
A. Lazicki
M. J. Lipp
B. Maddox
M. E. Manley
S. K. McCall
K. T. Moore
A. J. Schwartz
A. S. Sefat
R. F. Smith
A. P. Sorini
M. A. Wall
S. T. Weir
J. M. Zaug
Lehigh University
B. Kokoszka
K. Landskron
C. Liu
M. Mandal
P. Mohanty
M. Weinberger
Los Alamos National Laboratory
R. Chellappa
D. M. Dattlebaum
J. Han
Z. J. Lin
B. Nolan
E. B. Orler
J. Qian
D. Robbins
S. Sheffield
L. L. Stevens
N. Velisavljevic
J. Wermer
J. M. Zaug
J. Z. Zhang
R. F. Zhang
Y. Zhao
J. Zhu
Maquarie University, Australia
S. M. Clark
Massachusetts Institute of Technology
N. Ando
K. Catalli
S. H. Shim
McGill University, Canada
W. G. Minarik
McMaster University, Canada
P. A. Dube
Memorial University of Newfoundland, Canada
J. M. Hanchar
Muronan Institute of Technology, Japan
C. Sekine
I. Shirotani
Nancy Université, France
S. Lebegue

National Academy of Sciences of Ukraine
Y. A. Freiman
A. Grechnev
S. M. Tretyak
National High Magnetic Field Laboratory
T. Gebre
National Institute for Materials Science, Japan
M. Imai
N. Tsujii
National Institute of Standards and Technology
P. Gehring
Q. Z. Huang
X. Sha
H. Wu
National Research Council of Canada
D. D. Klug
National Synchrotron Radiation Research Center, Taiwan
N. Hiraoka
H. Ishii
K. D. Tsuei
New Jersey Institute of Technology
K. H. Ahn
H. Chen
Z. Chen
P. Gao
T. A. Tyson
T. Wu
New Mexico State University
B. Kiefer
North Carolina State University
J. Kang
C. Lee
M. H. Whangbo
Northern Illinois University
M. Frank
U. Patel
M. van Veenendaal
H. C. Watson
Z. Xiao
Northwestern University
K. A. Adams
C. R. Bina
D. M. Jurdy
S. M. Thomas
Oak Ridge National Laboratory
D. L. Abernathy
J. Bai
O. Delaire
M. A. McGuire
J. J. Molaison
A. F. Moreira dos Santos
N. Pradhan
B. C. Sales
A. S. Sefat
M. B. Stone
C. A. Tulk
Oakland University
Y. Wang
Ohio State University
G. S. Daehn
Oregon State University
A. E. Smith
M. A. Subramanian
Osaka City University, Japan
K. Murata
N. R. Tamil Selvan
H. Yoshino
Osaka University, Japan
F. Honda
Y. Nakamoto
K. Ohta
Y. Onuki
M. Sakata
R. Settai
K. Shimizu
H. Sugita
Okayama University, Japan
R. Eguchi
Palo Alto High School
T. L. Kao
Peking University, China
J. Chen
Q. He
X. Hu
S. Li
X. Liu
J. Tang
R. Tao
H. Wang
S. Wang
L. Zhang
Pennsylvania State University
S. Zhang
Polish Academy of Sciences
T. Palasyuk
Poolesville High School
P. N. Chen
Princeton University
J. A. Montoya
Renmin University, China
G. F. Chen
Z. Y. Lu
Rensselear University
P. Keblinski
J. Lian
S. Shenogin
Russian Academy of Sciences
A. Gavriliuk
I. A. Trojan
Rutgers University
S. W. Cheong
Y. J. Choi
K. Haule
S. Kim
G. Kotliar

Sandia National Laboratory
C. T. Seagle
A. L. Lima Sharma
P. A. Sharma
C. D. Spataru
J. D. Sugar
Seoul National University, Korea
H. I. Kim
S. K. Lee
S. Y. Park
Shanghai Institute of Micro-System and Information Technology, China
Z. Song
Shizuoka University, Japan
V. Mizeikis
Sichuan University, China
M. Chen
D. He
F.Peng
S. Wang
Simon Fraser University
A. A. Bokov
Z. G. Ye
Sincrotrone Trieste, Italy
G. Aquilanti
Smithsonian Institution
E. Cottrell
South China Institute of Technology
F. J. Jia
Z. X. Qin
L. Y. Tang
S. Yang
Southern University
J. Lei
S. Yang
Stanford University
C. Chen
Y. Cui
T. P. Devereaux
C. C. Kao
Y. Liu
H. Ma
C. Y. Shi
A. Vailionis
S. Wang
Y. Yang
S. C. Zhang
State University of New York – Stony Brook
Z. Chen
Z. Q. Cheng
B. Li
W. Liu
M. Ma
J. Parise
L. B. Skinner
Stony Brook University
S. E. Boulfelfel
B. S. Li
A. R. Oganov
L. Wang
Q. Zhu
Swineburne University of Technology, Australia
S. Juodkazis
Technische Universität Darmstadt, Germany
M. Andrade
D. Dzivenko
G. Miebe
R. Riedel
Technische Universität Munchin, Germany
S. Veprek
Tokyo Institute of Technology, Japan
K. Hirose
T. Komabayashi
Tokyo Metropolitan University, Japan
H. Sato
United States Army Research Laboratory
J. Ciezak-Jenkins
United States Geological Survey
I. M. Chou
Universidad Compultense de Madrid, Spain
M. G. Rabie
R. Sáez Puche
Universidad de la Laguna, Spain
J. López-Solano
A. Muñoz
P. Rodríguez-Hernández
Universidad de València, Spain
D. Errandonea
R. Lacomba-Perales
J. A. Sans
Università degli Studi di Milano, Italy
G. D. Gatta
Università Sapienza, Italy
E. Arcangeletti
M. Capone
P. Postorino
Università di Perugia, Italy
C. Petrillo
Universität Bayreuth, Germany
N. Dubrovinskaia
L. Dubrovinsky
D. J. Frost
A. Kurnosov
C. McCammon
Universitat Politècnia de València, Spain
O. Gomez
O. Gomis
F. J. Majon
Universität zu Köln, Germany
M. M. Abd-Elmeguid

Université de Toulouse, France
A. Corgne
Université du Littoral, France
E. Bychkov
Université Pierre et Marie Curie, France
D. Antonangeli
J. C. Chervin
G. Fiquet
A. Polian
University College London, UK
I. K. Robinson
University of Alabama – Birmingham
N. Brady
D. Hilton
J. Montgomery
G. Samudrala
S. A. Thomas
G. M. Tsoi
L. E. Wenger
University of Arizona
S. H. Evans
M. J. Origlieri
H. Yang
University of Calgary, Canada
S. Antao
University of California – Berkely
R. Jeanloz
K. Lutker
P. J. M. Monteiro
J. E. Oh
D. K. Spaulding
M. Wong
University of California – Los Angeles
R. W. Cumberalnd
R. B. Kaner
J. B. Levine
Z. Mao
R. Mohammadi
E. S. G. Rainey
S. H. Tolbert
B. E. Weaver
M. Xie
University of California – Pasadena
P. Asimow
University of California – San Diego
J. Hamlin
M. B. Maple
D. A. Zocco
University of California – Santa Cruz
E. Knittle
Q. Williams
University of Chicago
P. Dera
P. Eng
V. B. Prakapenka
T. Sakamaki
Y. Wang
T. Yu
University of Colorado – Boulder
D. A. Brown
J. R. Smyth
Y. Ye
University of Durham, UK
J. A. K. Howard
C. M. Robertson
University of Edinburgh, UK
G. J. Ackland
O. Degtyareva
E. Gregoryanz
C. L. Guillaume
R. T. Howie
M. Marques
M. I. McMillan
J. E. Proctor
T. Scheler
B. Tegner
University of Florence, Italy
F. A. Gorelli
M. Santoro
University of Illinois
D. Abdula
P. Braun
D. Ceperley
R. Conner
K. Esler
E. A. Friedman
Y. Fu
K. Kang
J. Kim
H. Kujiwara
A. Lagutchev
C. Lei
M. Losego
K. Nguyen
T. Ozei
M. Shim
D. Trinkle
X. Zheng
University of Kentucky
G. Cao
University of Koeln, Germany
H. Schneider
University of Maryland
N. P. Butch
C. Chen
Y. Kadry
K. Kirshenbaum
W. F. McDonough
J. Paglione
S. R. Saha
P. Syers
University of Michigan
B. Chen
M. Lang
J. M. Zhang
F. X. Zhang

University of Nebraska
H. Li
X. C. Zeng
University of Nevada – Las Vegas
D. Antonio
L. Bai
N. Bhattacharya
C. Chen
A. Cornelius
M. Galley
T. Hartmann
D. Hatchett
O. Hemmers
P. Kalita
R. Kumar
K. Lipinska-Kalita
Q. Li
Y. Liu
M. Nicol
M. Pravica
J. Robinson
J. Romann
H. Ruiz
A. Simon
O. Tschauner
J. Wojno
Y. Zhang
Y. Zhao
University of North Florida
L. Gasparov
Z. Kann
M. Lufaso
Z. Shirshikova
University of Saskatchewan, Canada
J. S. Tse
H. Wang
J. Yang
University of Science and Technology of China
L. Z. Cao
X. H. Chen
P. Cheng
X. F. Wang
J. J. Ying
Z. J. Xiang
University of South Carolina
T. Vogt
University of Tennessee
J. L. Musfeldt
University of Texas – Austin
J. G. Cheng
J. B. Goodenough
Z. Mao
J. S. Zhou
University of Tokyo, Japan
K. Komatsu
K. Matsubayashi
K. Mibe
S. Ono
Y. Uwatoko
University of Toledo
B. Chidester
University of Toyama, Japan
R. Higashinaka
T. Ikeno
Y. Isikawa
H. Sato
University of Tsukuba, Japan
S. Kojima
University of Washington
B. A. Mattern
J. I. Pacold
G. T. Seidler
University of Waterloo, Canada
A. Mailman
R. T. Oakley
S. M. Winter
X. Yu
University of West Georgia
M. Bishop
G. N. Chesnut
University of Western Ontario
Z. Dong
L. Liu
R. A. Secco
T. K. Sham
S. R. Shieh
Y. Song
W. Yong
K. K. Zhuravlev
University of Wisconsin – Madison
S. Jin
L. Li
S. A. Morin
Uppsala University, Sweden
R. Ahuja
Z. Konôpková
P. Lazor
C. Moyses Araujo
M. Ramzan
Virginia Commonwealth University
P. Jena
S. Li
Virginia Polytechnic Institute and State Universtiy
C. DeVreughd
J. Li
D. D. Viehland
VSB –Technical University of Ostrava, Czech Republic
A. Legut
Wake Forest University
B. Kolb
C. W. Matthews
J. G. O. Ojwang
T. Thonhauser

Washington State University
J. Y. Chen
R. P. Dias
M. Kim
B. A. Mattern
J. I. Pacold
G. T. Seidler
A. Sengupta
H. Wei
C. S. Yoo
Washington University – St. Louis
H. B. Banks
G. Fabbris
Williams College
A. S. Benjamin
A. Kung
Wuhan University of Technology, China
X. Hu
H. Huang
F. Jing
L. Zhang
W. Y. Zhao
Xiamen University, China
Y. Pan
Z. Sun
J. Zhou
Yale University
J. E. Panzik
C. Tomé
Yantai University, China
C. Zhang
Yonsei University, Korea
H. J. Hwang
J. H. Im
T. H. Kim
Y. J. Lee
Y. M. Lee
D. Liu
D. Seoung
Zhejiang University, China
J. Chen
J. H. Dai
M. Fang
J. Z. Jiang
L. J. Li
X. Ma
H. Wang
Z. A. Xu
D. Yang
Z. Zeng

3.5 Visitors to CDAC

Carnegie also receives many visiting scientists each year, who utilize laboratory facilities to prepare and perform experiments that would be impossible to do at their home institutions. Scientists from around the country and the world have visited **Carnegie** to take advantage of this program. Such visitors often make formal presentations, which enrich the scientific work of the group as a whole.

Visitors	Affiliation	Project	Date
A. Koleshnikov	Moscow State Academy	Hydrocarbons under extreme conditions with Alexander Goncharov	March 11-April 11, 2011
A. Gavriliuk	Institute for High Pressure Physics, Russian Academy of Sciences	Work with Viktor Struzhkin	March 21-April 22, 2011
K. Lokshin	University of Tennessee	Work with Viktor Struzhkin	April 13-16, 2011
Xiulan Jiang	Qingdao Technological University, China	Investigations of properties of liquids using Raman spectroscopy with Alexander Goncharov	April 21, 2011-August 21, 2011
Y. Wang	GSECARS	Work with Yingwei Fei	April 28-30, 2011
L. Burkemper	University of New Mexico	Element partitioning in the multi-anvil laboratory with Yingwei Fei	May 31-June 10, 2011
M. Ntam	Auburn University	Thermal conductivity of lower mantle minerals with Alexander Goncharov	July 5-July 31, 2011
Yuki Nakamoto M. Sakata T. Nakase	Osaka University	Work with Ho-kwang Mao and Takamitsu Yamanaka	July 5-August 3, 2011
T. Muramatsu	University of Houston	Work with Viktor Struzhkin	July 13, 2011

W. van Westrenen	Vriji University	Multi-anvil experiments with Yingwei Fei on the interior evolution of the Moon and Mars	July 11-22, 2011
M. Mandal	Lehigh University	Work with Yingwei Fei on high-pressure experiments using various meso-structured materials	August 2-31, 2011
H. Huang	Wuhan University of Technology, China	Melting behavior of Fe-O-S-Si under high pressures	August 26, 2011-August 25, 2012
S. Lovanov	Institute of Geology and Mineralogy, Russia	Work with Alexander Goncharov on the transformations that take place with light alkanes (C1-C5) under P and T relative to the Earth's mantle and experiments on the speciation of COH fluids with respect to mantle redox conditions	January 25-June 25, 2012
A. Palke	Stanford University	Work in multi-anvil laboratory with Yingwei Fei	March 27-April 4, 2012
P. Lazor	Uppsala University	Investigate thermal properties of materials in DACs, combining laser heating and finite element analysis, as well as performing low-temperature experiments with the PPMS system	April 13-26, 2012
A. Gavriliuk	Institute for High Pressure Physics, Russian Academy of Sciences	Work with Viktor Struzhkin	May 16-June 20, 2012
C. Knab	University of North Florida	Research on magnetite under high pressure with Viktor Struzhkin	May 22-June 12, 2012
A. Chanyshev	Novosibirsk State University, Russia	Work on deep carbon in the Earth with Alexander Goncharov	June 1-August 31, 2012
W. Zhou	Chinese Academy of Science	Exploring high pressure studies of nanomaterials and melting lines of simple molecules	August 20-31, 2012
W. Grochala	University of Warsaw, Poland	High pressure studies, resistivity measurements, and Ag (II) compounds with Viktor Struzhkin	September 24-28, 2012
A. Kolesnikov	The Russian State University of Oil and Gas	EOS measurements for ethane, propane and n-Butane using Brillion scattering and Raman and IR spectroscopies up to 20 GPa and 1000 K with Muhetaer Ahart & Maddury Somayazulu	November 6-December 23, 2012
A. Gavriliuk	Institute for High Pressure Physics, Russian Academy of Sciences	Work with Viktor Struzhkin	December 1-23, 2012

3.6 Carnegie CDAC Group Meetings for 2011-2012

The members of CDAC located at **Carnegie** meet several times a month to discuss their research and a brief talk is given by one of the members or by a guest speaker. In addition, members of the group will share recently published papers with their colleagues.

Speaker	Affiliation	Topic	Date
A. Karandikar	Carnegie	Methods to detect metal melting in DACs	January 7, 2011
Z. Liu	Carnegie	Superhard materials: Plans and Progress	January 14, 2011
J. Potter	Carnegie	Chemical equilibrium in hydrogenation reactions under elevated pressure	January 20, 2011
J. Hlinka	Czech Academy of Sciences	Oblique mode dispersion in $BiFeO_3$ by Raman scattering	February 3, 2011
J. G. O. Ojwang	Carnegie	High *P-T* studies of ammonia	February 4, 2011
C. Park	HPCAT	Paris-Edinburg cell development at HPCAT	March 15, 2011
A. Kyono	Carnegie	The influence of the Jahn-Teller effect at Fe^{2+} on the spinel structure at high pressure	March 25, 2011
D. Hummer	Carnegie	Crystal chemistry of Fe^{3+} in magnesium silicate perovskite and implications for lower mantle properties	April 1, 2011
C. Seagle	Carnegie	Conductivity of iron in Earth's core	April 15, 2011
Y. Wang	GSECARS	From solids to melts – development of the LVP program at GSECARS for understanding dynamic processes in the Earth	April 29, 2011
E. Gaillou	Carnegie	Pink diamonds: A tough past revealed	May 18, 2011
L. Burkemper	University of New Mexico	Molybdenum partition coefficients and planetary core formation	June 10, 2011
T. Yamanaka	Carnegie	Japanese island change with plate motion: Tohoku earthquake	June 10, 2011
B. V. Spitsyn	Russian Academy of Sciences	Origin and evolution of the CVD diamond	June 20, 2011
L. Zhang	Carnegie	Exploring Earth's lower mantle: Constraints from *in situ* XRD and quantitative chemical analysis	June 24, 2011
D. Popov	HPCAT	X-ray topography at 16-BM-B beamline: current status and possible applications	June 29, 2011
M. Ahart	Carnegie	Pressure induced structural phase transition in FeGa-alloy	July 1, 2011
T. Muramatsu	University of Houston	Low temperature resistivity measurements using DAC	July 13, 2011
L. Burakovsky	LANL	Inverse-Z method for phase diagram studies: Beryllium and magnesium as examples	July 26, 2011

A. Sengupta	Princeton University	Carrier dynamics to phase transitions: Exploring the nature of materials	July 29, 2011
K. Hernandez	California State University – Sacramento	Raman spectroscopic studies of the carbon dioxide-water system at high pressure	August 11, 2011
A. Benjamin	Williams College	EOS of the fluorinated copolymer Kel-F 800 to near megabar pressures	August 11, 2011
T. Liu	Howard Community College	Optical emission spectroscopy studies of MPCVD diamond growth	August 11, 2011
E. Stavrou	University of Ottawa	High pressure research: from polyamorphism to polymerism	August 15, 2011
S. Kulkarni	easyLab Technologies	Synthesis and characterisation of novel materials using high *P-T* techniques	September 6, 2011
O. Kurakevych	Institut de Mineralogie et de Physique des Milieux Condenses	Phase transformations and microstructure evolution of carbon-like and boron-rich solids under high *P-T* conditions	September 7, 2011
Y. Tian	LT Technologies, LLC	Microwave based technique for ultra-fast and ultra-high temperature thermal processing of materials and semiconductors	September 9, 2011
D. Hummer	Carnegie	Ionic moduli: A new theoretical framework for describing the compression of ionic solids	September 9, 2011
A. Laskin	AdlOptica GmbH, Germany	πShaper –Advanced refractive beam shaping optics	October 13, 2011
S. McMillan	Carnegie	Bridging the gap between static and dynamic compression: Approaching inertial confinement in DAC experiments	October 20, 2011
Amy Lazicki	LLNL	Phase diagram of shock- and ramp-compressed tin	October 28, 2011
L. Yang	Carneige	Melting of refractory metal rhenium in a DAC	November 4, 2011
O. Kurakevych	Carnegie	High *P-T* behavior of carbon-like and boron-rich solids	November 18, 2011
I. Naumov	Hewlett-Packard	1. Vortices in ferroelectric structures 2. Electronic structure and phase stability in V, Nb, and Ta under pressure	December 2, 2011
A. Epshteyn	Naval Research Laboratory	Air-stable reactive metal nanopowders from *in situ* sonochemical decomposition of metal hydrides	January 27, 2012
S. P. Tiwari	Center for Research in High Energy Materials, India	Density functional study of energetic materials	January 31, 2012
E. B. Gordon	Institute of Problems of Chemical Physics, Russian Academy of Sciences	New mechanism of impurities coalescence in superfluid helium	February 2, 2012

D. Sverjensky	Carnegie	Progress report on water properties at elevated temperatures and pressures	March 16, 2012
T. Yamanaka	Carnegie	Determining mineral names	March 23, 2012
A. Palke	Stanford University	Al- and Fe-substitution in $MgSiO_3$ perovskite: Paramagnetic interactions in NMR spectroscopy	March 30, 2012
E. Stavrou	Carneige	Correlation between Boston peak and first sharp diffraction peak under pressure, revisited	April 13, 2012
M. Manik	Lehigh University	Synthesis of quartz and coesite nanocrystals from periodic mesostructured silica at high pressure	April 19, 2012
S. Mandal	Michigan Technical University	Electron transport in nanoscale junction: A first principles investigation	May 3, 2012
W. Vos	University of Twente	Photonic band gap crystals: Islands of tranquility in a fluctuating vacuum?	May 11, 2012
B. Chen	University of Michigan	Rapid terrestrial core formation from *in situ* x-ray radiography and microtomography	May 18, 2012
S. Mikhail	Carnegie	Natural polycrystalline diamond: Beautifully ugly, chemically interesting, surprisingly overlooked	June 22, 2012
S. Gramsch	Carnegie	The Jahn-Teller effect: A clarification and some examples	June 29, 2012
S. Hunt	University College, London	Inferring the properties of $MgSiO_3$ post-perovskite from analogue materials	June 15, 2012
J. Mesa Garcia	Universidad EAFIT, Colombia	Learning through Fe isotopes: From planets to minerals	July 12, 2012
C. S. Yoo	Washington State University	Mbar chemistry: Novel states and transitions in simple molecular systems	July 23, 2012
J. Wollmershauser	Naval Research Laboratory	Multi-anvil press capabilities at the Naval Research Laboratory	July 31, 2012
C. Jin	Chinese Academy of Sciences	Pressure tuned new quantum states of correlated systems	July 31, 2012
G. Farfan	Stanford University	3d transition metal carbonates at high pressure	August 16, 2012
A. Chanyshev	V. S. Sobolev Institute, Russia	Hydrocarbons in the deep Earth interiors: Stability, decomposition, melting	August 24, 2012
S. Stefanoski	University of South Florida	Synthetic approaches in materials research: Crystal-growth and structure-property relationships of intermetallic clathrates	November 16, 2012
M. Sangwan	New Jersey Institute of Technology	Kinetics of elementary combustion reactions at elevated pressures and temperatures	November 27, 2012

3.7 2011 and 2012 SSAA Symposiums

The annual SSAA symposium, which is held in Washington DC, has served as a showcase for CDAC graduate students to present their work and to connect with other graduate students in the program. Highlighting the meeting is the student poster session (Fig. 64), in which CDAC students have been heavily represented. It is expected that all CDAC-supported students attend and present a poster, and over the past two meetings, we have had close to 100% attendance from CDAC students.

Figure 64. *CDAC students present posters during the 2011 and 2012 SSAA Symposiums in Washington, DC.*

CDAC Posters Presented at the 2011 SSAA Program Symposium

Al-Khatatbeh, Y., Mechanical strength of zirconia and hafnia phases, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Barkley, M., Classification and topology of hydrogen environments in hydrous minerals: An update, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Bi, W., High-Pressure Studies of Structure, Valence, and Magnetism in Europium Metal to 92 GPa, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Brown, K., Time-resolved emission spectroscopy of shocked materials, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Chang, Y. Y., Electronic spin transition of iron in dense hydrous magnesium silicate at high pressure, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Chidester, B., A high pressure study of the NH_3-H_2 system, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Fu, Y., E. Friedman, K. Brown, and D. Dlott, High pressure vibrational spectroscopy of molecular monolayers, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Holl, C., Single-crystal x-ray diffraction of bismuth sillenite (BSO) and its relevance for dynamic compression studies, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Hsieh, W. P., Development of metal film transducers for time-domain thermoreflectance at high pressures, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Kaercher, P., Texture of FeO during phase transition, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Kanitpanyacharoen, W., *In situ* laser and resistive heating techniques at high pressure in radial diffraction geometry, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, february 15-17, 2011).

Karbasi, A., Thermodynamics of several elements at high pressures, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Liu, J. and C. Lu, Sound velocity of iron and iron alloy measured at by high-energy resolution inelastic x-ray scattering (HERIXS), *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Mauger, L., Anharmonic behavior in Fe near the α-γ structural phase transition, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

McKiernan, K. and S. Amin, High-pressure Brillouin spectroscopy of basaltic glasses and characterizing pressure induced structural changes in glasses and liquids using NMR, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Munoz, J., Large softening of the phonon partial densities of states of C15 rare-earth-iron compounds, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Reaman, D., Viscosity constraints of Earth's inner core, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Uhoya, W., Collapsed tetragonal phae and superconductivity in 112 compounds, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Wang, J., Single-crystal elastic constants of SiO_2 under pressure -- A comparison between density functional theory and experimental techniques, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Wu, J., Synchrotron mossbauer spectra study of iron-based superconductor of $BaFe_2As_2$ at high pressure and low temperature, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

CDAC Posters Presented at the 2012 SSAA Program Symposium

Berg, C., Picosecnd time-resolved shock complression of energetic materials, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Brown, K. E. and W. Shaw, Optimizing laser-driven flyer plates for studying time-resolved emission of shocked materials, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Dunton, M., Structural transitions in silica and ligand capped silica nanoparticles under pressurse, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Finkelstein, G., New insights into high-pressure materials from synchrotron-based single-crystal x-ray diffraction, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Hohensee, G., High pressure thermal conductivity measurements of amorphous, crystalline, and alloy materials, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Hrubiak, R., Equations of state of group IVB transition metals (Ti, Zr, Hf) at high temperatures and pressures, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Kaercher, P., Two-phase deformation of lower mantle mineral analogs, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Kanitpanyacharoen, W., Preferred orientation and phase transformation of zirconium under high pressure and temperature, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Kavner, A., Fiber reinforced coposites under pressure: A case study in non-hydrostaticbehavior in the diamond anvil cell, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Lim, J., Studies of magnetism and superconductivity under extreme pressure, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Liu, J., Tandem magnetic transition in compressed Fe_7C_3, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Liu, J., Elasticity of iron alloys in Earth's inner core, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Lu, C., Elasticity of single-crystal pyrpe under high pressure-temperature conditions, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Mauger, Y., Polaron hopping in $LiFePO_4$ at elevated pressures and temperatures, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Meng, Y., Synchrotron XRD capabilities for research under extreme conditions at HPCAT, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Pray, J. M., Behavior of actinide-bearing materials under extreme conditions, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Uhoya, W., Simultaneous measurement of pressure evolution of crystal structure and superconductivity in $FeSe_{0.92}$ using designer diamonds, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Wang, Y., Crystal structure of graphite under room-temperature conpression and decompression, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Xia, Y., 16-ID-D high pressure spectroscopy at HPCAT, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Yang, J., Vibrational and elastic properties of ferromagnesite across the electronic spin pairing tansition of iron, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

3.8 CDAC Year 9 Review

The Year 9 CDAC Review took place on October 25, 2011 at the APS. Overview talks were given by Carnegie's **Russell Hemley**, **Stephen Gramsch**, **Ho-kwang Mao**, **Guoyin Shen**, and **Wenge Yang**. CDAC Academic Partners **Steven Jacobsen (Northwestern)**, **Dana Dlott (Illinois)**, **Yogesh Vohra (Alabama–Birmingham)**, and **Wendy Panero (Ohio State)** and CDAC Laboratory Partners **Jason Jeffries (LLNL)**, **Nenad Velisavljevic (LANL)**, and **Luke Shulenburger (SNL)** outlined their individual research programs to the review committee. In addition, 13 CDAC-supported graduate students attended the review and presented posters during a lunch-time poster session (Fig. 65).

Figure 65*. Scenes from the CDAC Year 9 Review.*

Posters Presented at the CDAC Year 9 Review:

Armentrout, M., Fiber reinforced composites under pressures: A case study in non-hydrostatic behavior in the diamond anvil cell, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Berg, C., Laser-driven shock compression of an explosive simulant monolayer, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Brown, K., Emission spectroscopy of shocked materials, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Chang, Y. Y., Electronic spin transition of iron in dense hydrous magnesium silicate at high pressure, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Dalton, D. A., Development of fast optical techniques for investigating extreme condensed states, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Hrubiak, R., Thermal conductivity of zirconium at high pressure and temperature in a laser heated DAC, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Kaercher, P., Crystallographic preferred orientation in FeO through the cubic-to-rhombohedral phase transition, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Kanitpanyacharoen, J., In situ laser and resistive heating techniques of Fe and (Mg,Fe)O at high pressure in radial diffraction geometry, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Mao, H. K., Advancing the HP-SR capabilities (invited), *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Mauger, L., Anharmonic behavior in Fe near the α-γ structure phase transition, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Munoz, J., Large softening of the phonon partial densities of states of C_{15} rare-earth-iron compounds, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Pigott, J., Microfabrication of controlled-geometry samples for the laser-heated diamond-anvil cell using focused ion beam technology, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Shen, G., HPCAT Program (invited), *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Townsend, J., Mbar-pressure synchrotron-IR of laser-heated materials in the diamond anvil cell, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Uhoya, W., Anomalous compressibility effects and superconductivity in 1-2-2 iron-base superconductors under high pressure, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Yang, W., HPSynC scientific and technique highlights (invited), *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

3.9 HPCAT Workshop on Advances in Matter under Extreme Conditions

CDAC Sponsored the HPCAT Workshop on Advances in Matter under Extreme Conditions (Fig. 66). The workshop was held from October 10-12, 2012 at the APS. Participants supported by CDAC funds (staff, partners, postdoctoral fellows, or students) are designated by an asterisk (*):

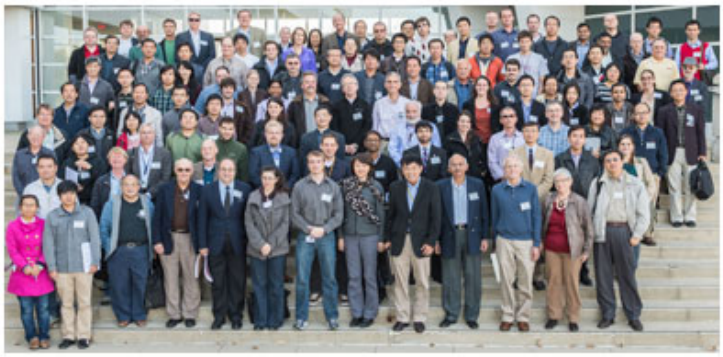


Figure 66. *Attendees at the HPCAT Workshop on Advances in Matter Under Extreme Conditions*

Workshop Highlights:

Plenary Session 1 – Chair: Christian Mailhiot

- **G. Brian Stephenson –** Welcome
- **Christian Mailhiot –** Charge of the Workshop
- **Ho-kwang Mao* –** HPCAT: An Integrated Facility for High Pressure Research
- **Eugene Gregoryanz –** Compressing the Group-I Elements

Plenary Session 2 – Chair: Thomas Duffy

- **Russell J. Hemley* –** New Opportunities in Compression Science
- **Brent Fultz* –** Inelastic X-Ray Scattering Studies of Phonons, Thermodynamics, and Kinetics of Materials
- **Yogendra Gupta –** Dynamic Compression Science at APS: Scientific Challenges and Research Opportunities

Plenary Session 3 - Chair: David Funk

- **Maddury Somayazulu* –** Novel Xenon Chemistry with a Diamond Anvil Cell
- **Per Söderlind –** Electron Correlation and Magnetism in f-Electron Metals under Pressure
- **Joseph Bradley –** Understanding f-Electron Itinerancy and Magnetism Using Volume Collapse
- **Daniel Hooks –** Explosives Science

Break-out Sessions

- **Panel 1: Structure, bonding and thermodynamic properties reaching 0.5 TPa and beyond**
  Chairs: Thomas Duffy*, Stanimir Bonev
  Panelists: Reinhard Boehler, Brent Fultz*, Carl Greeff, Eugene Gregoryanz, Richard Scalettar
- **Panel 2: Time-dependent transformations and off-Hugoniot processes**
  Chairs: William Evans, Shengnian Luo
  Panelists: Michael Armstrong, Jing-yin Chen, Eric Chronister, Daniel Hooks, Nenad Velisavljevic, Wenge Yang*
- **Panel 3: New materials: Discovery and applications**
  Chairs: Jonathan Crowhurst, John Tse
  Panelists: Barbara Lavina, John Moriarty, James Schilling*, Viktor Struzhkin*
- **Panel 4: Novel states of matter and new chemistry**
  Chairs: Dana Dattlebaum, Andrew Cornelius
  Panelists: Valentin Iota, Yue Meng*, Artem Oganov, Maddury Somayazulu*, Philip Sterne
- **Panel 5: Mechanical and transport properties of materials** *Chairs:* Yusheng Zhao, Hans-Rudolf Wenk*
  Panelists: Jon Almer, Joel Bernier, Changfeng Chen, Yanzhang Ma, Dmitry Popov*, Yanbin Wang
- **Panel 6: Liquid and amorphous materials**
  Chairs: Chris Benmore, Howard Sheng
  Panelists: Eric Chisolm, Malcolm Guthrie, Magnus Lipp, Changyong Park*, Chris Tulk
- **Panel 7: Advanced technologies and instrumentation**
  Chairs: Chi-chang Kao, Stanislav Sinogeikin
  Panelists: Ercan Alp, Kevin D'Amico, Tim Graber, Vitali Prakapenka, Paul Chow*, Jesse Smith*

Poster Session

- Poster cameo introductions – Chair: Stanislav Sinogeikin*

3.10 Workshop Explores NIF User Science Opportunities

CDAC scientists participated in a workshop entitled "Basic Research Directions for User Science at the National Ignition Facility (NIF)," from May 10-12, 2012 in Arlington, Virginia. The purpose of the workshop was to explore new scientific opportunities that will be possible with NIF, the world's largest and most powerful laser, which is located at **LLNL**. The workshop was convened by **John Sarrao (LANL)**, **Kimberly Budil (LLNL)** and **Michael Wiescher (University of Notre Dame)**. Scientific areas that will benefit from the capabilities of NIF include Laboratory Astrophysics, Nuclear Physics, Materials in Extremes and Planetary Physics, and Beam and Plasma Physics.

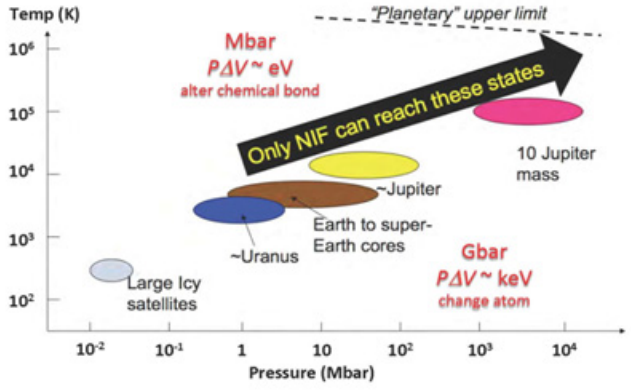


Figure 67. *The range of interior pressures and temperatures of classes of planets, and the corresponding effects of the compression on bonding energies of the component materials.*

Within each topical area, panelists summarized the status of the field and proposed opportunities for new and groundbreaking science. CDAC Director **Russell Hemley** chaired the Materials at Extremes and Planetary Physics panel and discussed the importance of NIF to understanding atomic and molecular interactions at the most fundamental level. States of matter approaching the Gbar pressure range will be possible with NIF, states in which the very nature of matter is unknown (Fig. 67). This will lead to increased

understanding of key problems such as the nature of materials strength, the origin and evolution of planets, and the process of thermonuclear fusion. CDAC participants in the Materials panel included academic partners **Tom Duffy** and **Raymond Jeanloz**, **Carnegie** staff scientist **Alexander Goncharov**, steering committee members **Rip Collins** and **Marcus Knudson** and advisory committee member **Yogendra Gupta**. The Materials panel also included **Paul Loubeyre**, **Sarah Stewart-Mukhopadhyay**, **Alfredo Correa**, and **Justin Wark**.

Integrating results from static and dynamic compression measurements for stockpile stewardship science has been a key goal of the CDAC program since its inception in 2003. With this outstanding new opportunity for advances in the field of extreme conditions science becoming available in the near future, CDAC will work to facilitate the coordination of the emerging user community and help to develop key scientific directions. For the first round of user science experiments at NIF, a **UC Berkeley-Carnegie** collaboration has been awarded time for work on hydrogen and hydrogen-containing materials at extreme conditions.

4. TECHNOLOGY DEVELOPMENT

Technical development is critical for advancing the frontiers of high *P-T* research, and within CDAC, improvements in many types of experimental methods are pursued. At **HPCAT**, continuous upgrades of equipment and techniques headline the CDAC effort in this area, but a number of impressive technical developments have occurred in the laboratories of our academic partners as well. In this section, we outline some of the technology development efforts that have taken place in the Center during 2011-2012.

4.1 Technical Improvements at HPCAT

The objective of **HPCAT** is to provide a state-of-the-art user facility for advancing fundamental knowledge of materials behavior in a broad range of environments, such as pressure, temperature, radiation, and deviatoric stress, including both static and dynamic phenomena. The integrated **HPCAT** facility allows for extreme conditions studies in: (1) structural determinations at various scales from amorphous, nano-, polycrystalline, single crystal, to microstructures of composite materials, (2) measurements of phonon dynamics, charge dynamics, and electronic and spin states of metals, alloys, oxides, nitrides, hydrides, new superconductors, and new superhard or other super-durable materials, (3) *in situ* measurements with high spatial resolution (1-3 μm) and high temporal resolution (down to 100 ps). Investigations of structure, equations of state, and electronic and magnetic properties provide critical data for code validation and tests of fundamental theory. The measured "structure-property" correlation helps to establish predictive models for development of new materials and new applications. **HPCAT** has continued to stay at the leading position in the world, and is the most productive sector at the APS in terms of the number publications in "high-impact" journals as well as the total number of publications. In the past year, we have successfully commissioned the newly-installed canted undulator configuration and associated beamline optics, including two new monochromators, and made them fully operational for general users; we have enabled two new high-pressure x-ray techniques and further enhanced the three existing high-pressure x-ray techniques; and we have expanded supporting equipment critical for high pressure research.

Highlights of Recent Facility Enhancements and Technical Developments at HPCAT

- **Canted undulator upgrade completed –** Two undulators in canted mode (Fig. 7) were successfully installed in October 2011. In the past

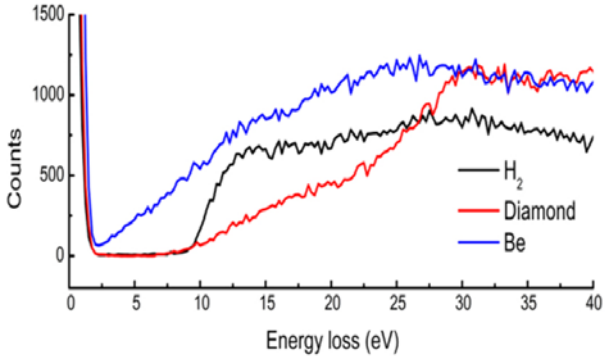


Figure 68. *Clear inelastic x-ray scattering signals of H_2 observed at high pressures using a diamond anvil cell.*

year, we have commissioned all the matching optics including two monochromators in the beamlines and completed the canted undulator upgrade project in time. The enhanced beamlines have been fully operational since November 2011. The canted operation provides two completely independent beamlines for high-pressure spectroscopy (16-ID-D) and diffraction (16-ID-B), respectively. The independent operation also allows for further optimizing x-ray optics and hutch instrumentation, providing increased flux at the sample position by an order of magnitude, as well as extended x-ray energies with scanning capability, which is critical for the spectroscopy beamline, and enhanced position and energy stability of x-ray beams.

- **Polycapillary optics improves signal/background ratios –** One of the major issues for inelastic x-ray scattering measurements in DACs is the parasitic scattering from the gasket and diamonds. Because of the relatively small inelastic scattering cross-section from the small sample, and large scattering volumes of the diamond and gasket as the beam enters and exits the cell, the desired inelastic scattering signal from the sample often rides on top of a large background. To improve the signal to background ratio for a cleaner measurement, we have replaced our collimation slit with polycapillary optics to improve discrimination of the scattering from the signal from that of the DAC. Although the polycapillary efficiency at 10keV is ~15%, the confocal geometry improves the signal-to-noise ratio, especially for studies of electronic excitations close to the elastic line. A large solid angle can be measured with a single analyzer. Additionally, the polycapillary optics allow for a proper measurement of the momentum transfer of the scattered photons. We have measured the inelastic scattering from H_2 at 10 GPa using an ~70 μm opening collimation slit and polycapillary optics for comparison (Fig. 68). There is a remarkable improvement in the signal/background using the polycapillary optics. The provides good depth and improves signal/background ratio by a factor of 5-10 in IXS measurements.

- **Comprehensive characterization of liquids at high pressure –** We have established a capability for comprehensive characterization of melt/liquid properties, allowing users to study structure (by XRD), density (by absorption measurement s), elasticity (by ultrasonic interferometry), and viscosity (by radiographic imaging) at high pressure and temperature. The developed system is based on a Paris-Edinburgh cell (PEC) installed at the 16-BM-B station. The PEC provides a large sample size (1-2 mm) and can be resistively heated to high temperatures (uniform temperature up to 2700 K). The PEC program at **HPCAT** provides a unique facility in the U.S. for comprehensive studies of liquids under high pressure. Very recently, the falling sphere viscosity measurement has been developed using x-ray radiography with a high-speed camera (> 1000 frame/second, Fig. 69), which enables investigation of the viscosity of not only highly viscous melts such as silicate or oxide melts, but also low viscosity liquids and fluids such as H_2O and CO_2 and liquid metals (around 1 mPa s or less at ambient pressure).

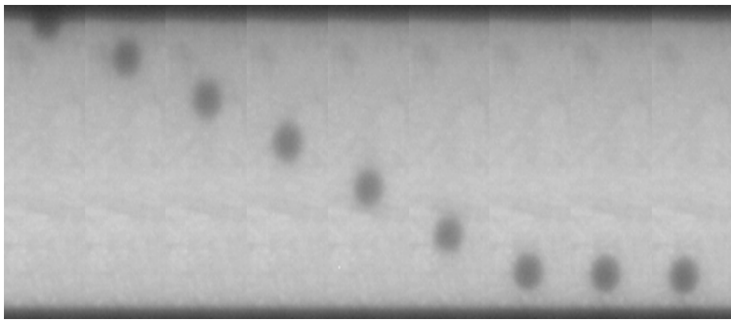


Figure 69. *Falling Pt-sphere images in liquid KCl at 6 GPa recorded by x-ray radiography at a frame rate of 2000 fps.*

- **Pulsed laser heating system –** The laser heating system at **HPCAT** has been significantly modified and improved for *in situ* studies of materials at high-pressures and high-temperatures. The pulsed laser has been synchronized with the incident x-ray beam (by x-ray chopper), temperature measurement (by CCD detector gating), and XRD (by using a Pilatus detector). Short-pulsed heating duration down to 100 ms can be applied to materials at high pressures for investigating dynamic phenomena, transport properties, and phase transition kinetics. In addition, the newly-developed capability opens opportunities in expanding the achievable *P-T* range, by recording materials properties in a time-resolved manner using the pulsed laser system. Established at 16-ID-B eight years ago, this technique has evolved in its sophistication and effectiveness, and has been a highly demanded, heavily used and productive experimental technique. Among recently established new

capabilities, the mirror-pinhole setup (Fig. 70) helps to directly observe the temperature sampling area on the heating spot; *in situ* variation of laser heating spot size (flat top area from 5 to > 60 microns, FWHM from 10 to >120 microns) allows for optimal heating areas required by various experiments. These developments provide new opportunities in several areas of research including *P-V-T* EOS and high-pressure melting.

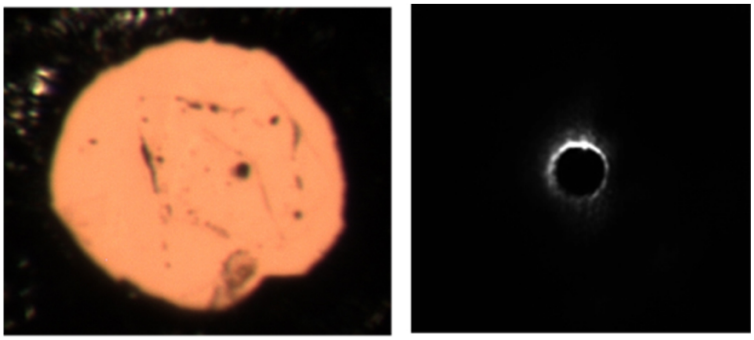


Figure 70. *Left: a Pt sample ball of 5 mm in size. Right: the mirror-pinhole setup for ensuring precise alignment of x-ray beam and heating spot.*

- **High resolution in XRD –** The angular resolution of high-pressure powder XRD at the 16-BM-D beamline has been improved up to $\Delta q/q \sim 10^{-3}$ by using a Pilatus 100K detector on the rotating 2-circle diffractometer arm (Fig. 71). The powder diffraction patterns from a NIST CeO_2 standard obtained using the 172 µm fixed-size pixel arrays located at ~500 mm distance showed roughly three times better angular resolution compared to those obtained with an IP or CCD detector at ~300 mm distance, with typical 30 keV x-ray energy. For the collection of a full diffraction pattern, multiple diffraction images are collected at discrete 2θ angles and stitched together with proper geometric corrections to be integrated into a consistent diffraction pattern. To minimize the misalignment of the diffractometer center between different 2θ angles, a heavy rotation stage is adopted, but with a light weight arm for the detector mount. The improved angular resolution benefits studies of low symmetry materials, samples with multiple phases, and subtle structural changes induced by magnetic or electronic transitions.

- **High-efficiency emission spectroscopy –** To improve the efficiency of XES experiments, in addition to the on-going project to implement more analyzers to the current setup, **HPCAT** has commissioned and used both a miniature x-ray emission spectrometer (miniXES) and x-ray emission spectrometer with polycapillary optics in collaboration with researchers from **University of Washington** and **LLNL**. The miniXES spectrometer for the Pr $L_{\alpha 1}$ emission line, based on a coarsely diced approximation of the Johansson optics, contains six small flat Ge(331) crystals placed close to the sample, a spatial filtering aperture and a low-noise x-ray position sensitive detector (Pilatus 100K). The overall energy resolution of the spectrometer is ~1.3 eV and the spectrometer has a total solid angle equivalent to six traditional spherically bent 1-meter radius, 4-inch crystal analyzers. The polycapillary optics can collect a solid angle as much as 16 degrees with a focus length ~8.5 mm. Combined with the flat Si crystal as the analyzer, the overall efficiency is ~4-5 times better.

- **Enabling the white beam Laue technique for high pressure research –** An experimental setup dedicated to the Laue technique is being commissioned at 16-BM-B. The high-pressure Laue technique can provide information on texture of polycrystalline materials, strain, dislocation arrangements, domain structure, and slip systems of single-crystals. The x-ray beam is focused down to 5-10 μm^2, with a typical energy range of 5-70k eV. A Si-111 channel cut monochromator provides a monochromatic beam of 40 keV, which operates in exchangeable manner with the white beam in order to get d-values of selected diffraction spots. Recent commissioning on the shape memory material Ni_2MnGa shows promising results of tracing the defect evolution as a function of *P-T* conditions (Fig. 72). The use of a white beam provides a large reciprocal space coverage and eliminates the need for

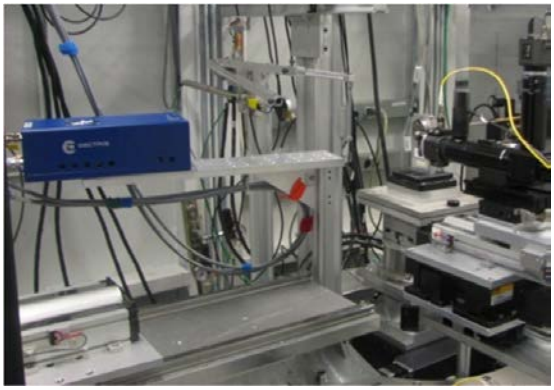


Figure 71. *The setup at 16BM-D for high resolution experiments in x-ray diffraction.*

rotating samples. This technique has great potential for studying materials deformation and defect evolution in a time-resolved manner.

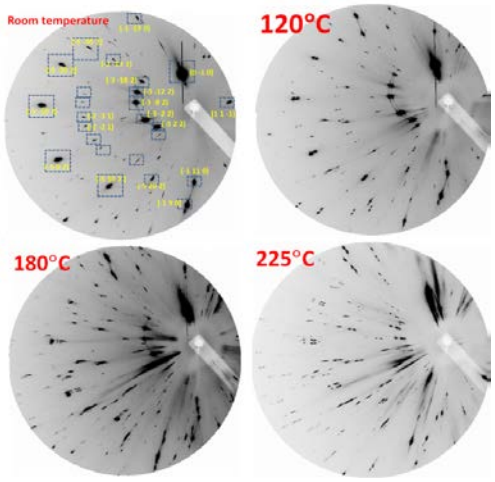


Figure 72. *Phase transitions and defects in Ni_2MnGa at high temperatures. Orthorhombic cell: a=4.276(5) Å, b=20.93(2) Å, c=5.397(7) Å.*

- **Supporting equipment –**

New Pilatus Detector 1M-F – The new detector is mainly stationed at 16-ID-B, but can be used at other **HPCAT** beamlines as needed. It has a number of unique characteristics including absence of readout noise and dark current (zero background), extremely sharp point spread function smaller than one pixel, high dynamic range of 20 bits, short readout/dead time of 2.3 ms and very high frame rates up to 130 Hz with shutterless operation and energy resolution. The unique characteristics of the PILATUS 1M-F detector open the door to many novel methods and advanced data collection strategies and enables a whole family of new types of experiments. For instance, the fast readout and high frame rates allow rapid, non-stop data collection in dynamic experiments such as fast EOS measurements, and high-speed pressure ramp and high strain rate experiments, which fill the gap between static and shock experiments. The detector also allows fast stroboscopic diffraction measurements with pulsed laser heating and piezo-modulated pressure experiments with discrete binning of ultrashort diffraction images based on pressure or temperature. The short readout time and high frame rates, combined with higher resolution, enable high throughput data collection and optimized beamline efficiency. As an example, the fast readout and high frame rates allow rapid non-stop 2 or 3-dimensional grid scanning and sample characterization (*e.g.* 2D and 3D diffraction tomography). The new detector also offers a real breakthrough in fast high-resolution single crystal data collection by allowing one-sweep, non-stop single crystal measurements. Due to the very short readout time of 2.3 ms, all high speed and high quality single crystal diffraction data can be collected during a single, continuous rotation, eliminating the shutter and acceleration/deceleration of the rotating motors as sources of error.

Cryostat project – Continuous developments have been made for various cryostats to be compatible with high-pressure single crystal diffraction, high-pressure XES, high-pressure NFS, and high-pressure inelastic x-ray scattering.

Remote pressure control – The developed remote control systems have now been digitized and can be controlled from beamline computers. These systems are not only used for serving **HPCAT** users, but many high pressure users around APS and beyond.

Fast loading or unloading in pressure control – Several pressure cells coupled with piezo controlled systems have been designed. The piezo-driven cell will allow for fast pressure ramp or drop at kHz rates. We also have developed a fast diaphragm-driven system for pressure control at a rate of a few Hz. These newly developed cells will be used together with the new Pilatus detector and the pulsed laser heating system for studying materials behavior in time-resolved measurements.

Glove box with manipulator – We have purchased a new glove box for handling samples that are environment-sensitive. The glove box is equipped with a micro-manipulating system, which greatly improves the sample loading quality in preparing micron-sized samples inside high pressure devices.

4.2 Next Generation Extreme Conditions Science at the APS

HPCAT has pioneered the use of third-generation synchrotron radiation to address problems in extreme conditions materials science. Designed in 1998, **HPCAT** has at this point uniquely developed and integrated multiple techniques at a single sector to advance multidisciplinary high *P-*

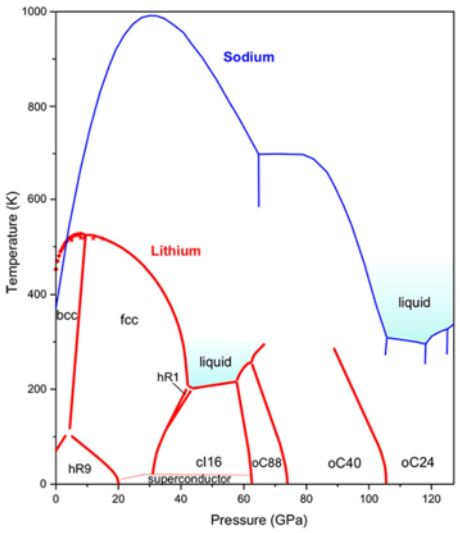


Figure 73 *. Complexity in "simple" metals. Phase diagrams of lithium (red) and sodium (blue).*

T research (https://hpcat.gl.carnegiescience.edu). Within five years of its construction and commissioning, **HPCAT** surpassed all high-pressure synchrotron radiation facilities in the world in terms of scientific output and emerged as one of the most productive sectors at the APS. Fourteen years of exploration at **HPCAT** have guided the direction of extreme conditions research. Moreover, **HPCAT** has made significant contributions to stockpile stewardship science, and advanced the NNSA science mission.

At the same time, our facility is aging and facing steep competition from newly established high *P-T* beamlines in Europe and Asia that have adopted the **HPCAT** model. We have reached a critical stage for a major upgrade to stay at the cutting edge. The proposed upgrade will accomplish two goals at the same time: (1) advancing to the next generation of high *P-T* synchrotron science, (2) expanding deliverable beam time for increased user activities.

Current Capabilities at HPCAT – During the past decade, **HPCAT** has developed an arsenal of high *P-T* synchrotron radiation techniques. These tools, integrated with hydrostatic or uniaxial compression, laser heating, and cryogenic cooling, have enabled users' investigations of extreme *P-T* structural, vibrational, electronic, and magnetic properties that were not possible a decade ago. The current **HPCAT** capabilities can be summarized as follows:

- *Probing structures at various scales in space and time*: By using high *P-T* XRD and x-ray imaging techniques, structures of materials [amorphous, (nano-) crystalline, and microstructure] can be determined *in situ* at high *P-T* and high or low temperatures (Fig. 73). Fast imaging and diffraction measurements can be performed at the sub-millisecond level for high *P-T* samples to be recorded with time-resolved information such as materials transport properties, metastability, and transition kinetics (Fig. 74).

- *Measuring electronic, phonon, and magnetic properties* at high *P-T* and high or low temperatures by a variety of high *P-T* x-ray spectroscopy techniques pioneered at **HPCAT**.

- *Pressures up to 350 GPa and temperatures from 4-6000 K*: With a typical probing size of 3-5 μm, the highest pressure reaches to a plateau of 300-400 GPa. Use of cryostats allows for exploring properties of materials at temperatures down to 4K. With laser heating, we can reach temperatures over 1 eV (>11,000 K); however, measurable temperatures are within 6000 K

The **HPCAT** facility has four simultaneously operational beamlines with specialized x-ray optics and high *P-T* synchrotron radiation instruments in nine stations. The essential operation budget is required to support a team of beamline staff and to cover the maintenance and outreach cost and minor development projects. **HPCAT** is widely used by the high *P-T* community with >500 person-visits per year, among which >60% are graduate students and post-doctoral researchers. **HPCAT** is an important educational

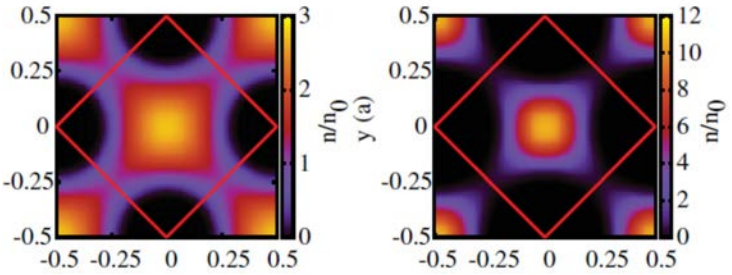


Figure 74 *On the approach to close packing, the electron density develops maxima at positions in the interstitial cell that are maximally distant from the neighboring spheres.*

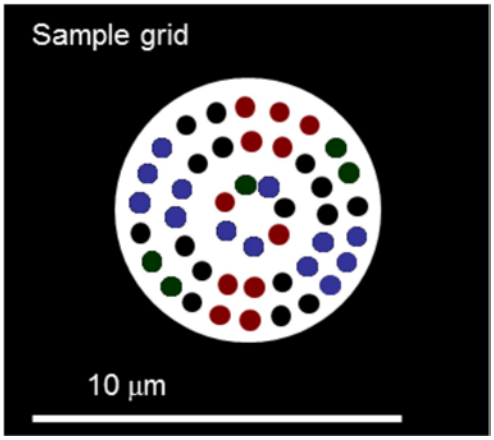


Figure 75. *Wtih a nanofocused x-ray beam, combinatorial studies and simultaneous pressure calibration experiments may be carried out on many samples at the same time in the diamond anvil cell.*

and training ground for the next generation of extreme conditions scientists. In addition to numerous reports to the DOE programs, there are >1.5 peer-reviewed papers published per week, among which >23% appear in high profile journals with impact factors ≥ *Physical Review Letters*.

HPCAT Upgrade – Next Generation High P-T Research – Further advancement is waiting for the integration of a battery of high *P-T* synchrotron radiation techniques to meet new challenges in high *P-T* science and technology with the new opportunities including the APS Upgrade, the potential NNSA-sponsored center at the APS, and novel high *P-T* synchrotron radiation techniques that have recently become feasible and practical.

- *Advancing static high pressure limits to >500 GPa or higher*, far beyond the current capability of ~350 GPa, will redefine the scope of high *P-T* research and enable studies in entirely new regimes of physics. We have limited understanding of structure and bonding in condensed matter at very high compressions. A general predictive theory is still lacking. Current observations are based on phenomena observed to pressures of 300-400 GPa. What happens at higher pressures? There are numerous challenges including the quest for the metallic fluid hydrogen for deeper understanding of the nature of matter, and the understanding of a new type of chemical bonding observed in alkali metals at significant compression.

- *Transformational advances for precision and accuracy by improving spatial resolution*: One order of magnitude improvement in spatial resolution will enable quantifications of microstructure and grain-to-grain interactions under pressure, precise determinations of equations of state and pressure calibration, combinatorial studies of a large array of samples (Figs. 75, 76), density determinations for amorphous/liquid materials, and isolation of a μm-size single crystal from a polycrystalline aggregate. A wide range of discoveries in basic physics is expected, including pressure-induced superconductivity, ferroelectricity, colossal magnetoresistance, phonon softening, Fermi-surface nesting, *d*-electron spin pairing, *f*-electron delocalization, insulator-metal transitions and the reverse.

- *Enabling studies in a time domain between static and dynamic techniques*: Complementary to dynamic compression science, which typically deals with events at ns-ps-fs intervals, the **HPCAT** upgrade will improve temporal resolution by 2-3 orders of magnitude, enabling new time resolved x-ray capabilities with time resolutions down to sub-microseconds. This time resolution covers the gap between "static" and "dynamic" and is important for studying the kinetics and mechanisms of physical and chemical processes. The enhancement is critical for enabling the studies of transport properties at high *P-T* (diffusivity and conductivity) and kinetic processes (melting, phase transitions, and metastability). It will also enable new ways of studying compression behavior of materials at a fast

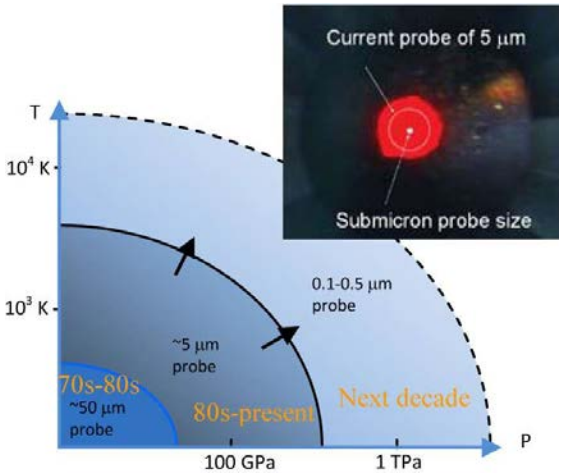


Figure 76. *Technical improvements that may be realized with the HPCAT upgrade include a decreasing size of the x-ray beam with dramatically increasing maximum static pressures, which will allow mapping of material properties on the nanoscale.*

rate of strain change. For example, pressure-volume (or other properties) relations can be measured from ambient pressure to over 500 GPa within a second by quickly ramping pressures by, *e.g.,* using a piezo-driven DAC and a new pixel array detector (Pilatus).

A *three-phase* approach is proposed for the **HPCAT** upgrade (Fig. 77). We are currently in Phase 1, which involves the installation of canted undulators (funded by the ARRA) and matching heat load optics such as monochromators and primary slits and focusing devices, megabar high *P-T* spectroscopy, and advanced detectors. In Phase 2, we propose to have a major source enhancement (APS-U), enable sub-μm probes (diffraction and spectroscopy) and 30-*n*m resolution x-ray microscopy. While enhancing the spatial resolution, we will also make effort on depth resolution techniques for significant improvement in signal-to-noise ratio. Thus, together with advanced detector technology, we will have 2-3 orders of magnitude improvement in temporal resolution in high *P-T* XRD and high *P-T* x-ray spectroscopy. In Phase 3, the developments will be mainly in the areas of high *P-T* coherent diffraction imaging and x-ray scanning microscopy as well as the continuous developments in time resolved techniques and advanced detectors.

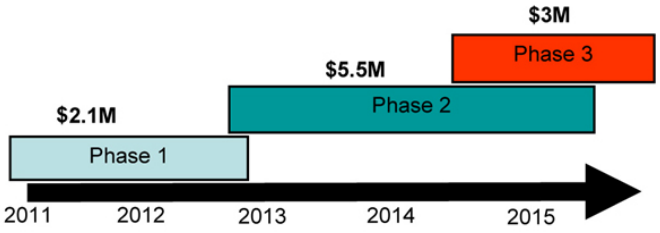


Figure 77. *Proposed scheduling of the HPCAT upgrade.*

A total of $10.6M is needed for the **HPCAT** upgrade over next six years, after considering the recent funds of $1.02M for advanced monochromators from NSF-MRI and 30% matching funds from **Carnegie** (see below). The current pending funds include a contingent project in the APS-U ($2M for sub-μm probes for Phase-2).

Governance Model – The **HPCAT** program has been supported by four member groups through funding from DOE-NNSA (75%) and DOE-BES (25%), including **Carnegie** (managing member), CDAC, **LLNL**, and **UNLV**. The governing body is the **HPCAT** Executive Council (HPC) consisting of group leaders from all member groups (executive director **Ho-kwang Mao**, along with **Russell Hemley**, **William Evans**, and **Yusheng Zhao**). The HPC committee meets every other month. A Technical Advisory Committee was established in 2006. Current members include **Chi-chang Kao**, **Mark Rivers**, **Wolfgang Sturhahn**, **Martin Kunz**, and **Deming Shu**. The **HPCAT** program is managed by director **Guoyin Shen**.

A new model is currently being implemented. In this new model, HPCAT is funded through a new NNSA cooperative agreement with **Carnegie** that simplifies the funding structure of **HPCAT** and takes advantage of the low "off-site" overhead rate of **Carnegie**. The new model will open a number of new opportunities that include increasing participation at **HPCAT** by scientists from all three NNSA laboratories, complementing and enhancing the SSAA program for training the next generation of scientists and engineers for the NNSA mission, enhancing the coordination with other programs at the APS (*e.g.*, DCS), and paving the way for establishing a central program at the APS for extreme conditions science for NNSA that will support the decadal facilities goals of the NNSA laboratories outlined in their roadmap.

With this new model, **HPCAT** will continue to provide an enabling platform for advancing fundamental knowledge of the behavior of materials central to the NNSA science mission in a broad range of environments, such as pressure, temperature, deviatoric stress, laser, and x-ray radiation. The **HPCAT** partners (Carnegie, CDAC, UNLV, and NNSA laboratory scientists) represent the leading high-pressure research groups in the U.S. and will continue to be the main body of the **HPCAT** user community. Meanwhile, the new model will allow the engagement of a still broader user community, including an expanded NNSA laboratory user base.

NNSA Center for Extreme Conditions Science at the APS – Extreme conditions science is now one of the major thrusts at several APS-operated beamlines, owing in part to the strong support by NNSA at HPCAT. The addition of DCS will bring the expertise and the user community in

dynamic compression. The new **HPCAT** model and the proposed upgrade will enhance the coordination of various programs at the APS, for example, by proper cost-sharing for Grand Challenge projects at multiple beamlines, beam-time allocation for complementary information and feasibility tests for DCS, and sharing large or expensive equipment (*e.g.*, detectors). With equipment that already serves users beyond **HPCAT**, the upgrade will establish a more comprehensive facility to support the NNSA science mission. The synergy between DCS and other APS beamlines will lead to a unique center for extreme conditions science at the nation's most brilliant hard-x-ray synchrotron source.

Summary – The **HPCAT** upgrade will take full advantage of the facility-wide APS upgrade for unmatched brilliance and will develop matching optics and novel integrated techniques, which will significantly improve both spatial and temporal resolution and provide superior tools for the community to lead the next level of development in extreme conditions science. In addition to traditional "static" or "dynamic" experiments, the **HPCAT** upgrade will provide novel x-ray capabilities covering a time domain that fills the gap between "static" and "dynamic" compression. Furthermore, the enabling platform with the upgrade for advancing fundamental knowledge of the behavior of materials will provide an important opportunity for training the next generation of scientists for work in this important area of research.

4.3 Infrastructure Development at Carnegie and Academic Nodes

Time- and Angle-Resolved XRD for Single Event Reactions – Understanding the dynamic response of a solid under extreme conditions of pressure, temperature and strain rate is a fundamental scientific quest and a basic research need in materials science. Specifically, obtaining an atomistic description of structural and chemical changes of solid under rapid heating and/or compression over a large temporal, spatial and energy range is challenging but critical to understanding materials stability or metastable structure, chemical mechanisms, transition dynamics, and mechanical deformation. In this regard, developing time-resolved XRD applied to single-event dynamic experiments is timely and synergistic to many proposed activities centered at third- and fourth-generation light sources.

In collaboration with scientists at **HPCAT** and the High Pressure Physics Group at **LLNL**, **Choong-shik Yoo** and his group at **Washington State University** have recently used CDAC beam time to develop a novel time- and angle-resolved XRD method. This technique is capable of probing structural and chemical evolution during rapidly propagating exothermic intermetallic reactions between Ni-Al multilayers and metal combustion.[106-108] The system utilizes monochromatic synchrotron x-rays and a two-dimensional (2D) pixel array x-ray detector in combination with a fast-rotating diffraction beam chopper, providing a time (in azimuth) and angle (in distance) resolved XRD image continuously recorded at a time resolution of ~30 ms over a time period of 3 ms. Multiple frames of the resulting images can also be obtained with time resolutions between 30 and 300 ms over three to several hundreds of ms (Fig. 78). The present method is applicable to a wide range of dynamic experiments to study both single event phenomena of solids under thermal, electric or mechanical impact conditions and non-single event changes using dynamic-DAC and high frequency pulsed lasers. The team is now furthering the development of this technique for studies of non-single event phenomena at extreme conditions with even faster time resolution.

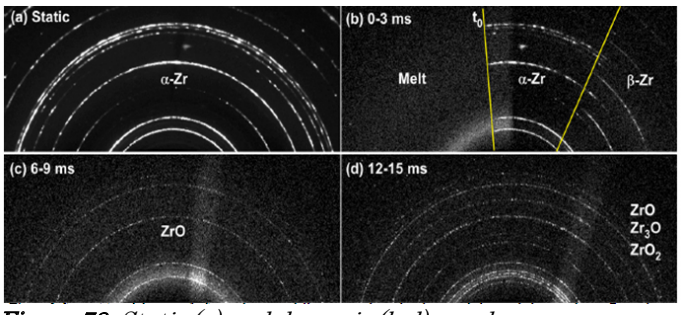


Figure 78. *Static (a) and dynamic (b-d) powder x-ray diffraction probing the phase and chemical changes during Zr combustion in air. These images were obtained with a time resolution of 45 ms for each 3 ms long combustion period. The yellow straight lines in (b) signify the onset of the pulsed heating (to) and the a-to-b Zr phase transition. Note that the various oxides are formed at different stages of combustion.*

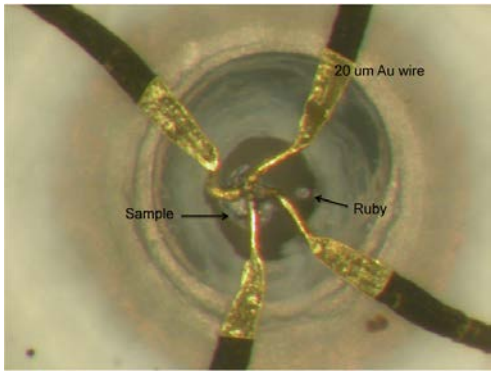


Figure 79. *Reflected-light photograph of diamond-anvil cell where the Pb sample has been spot-welded to four Au wires for resistivity studies in a fluid pressure medium.*

Magnetic Measurements in the DAC – A major disadvantage to using a diamond-anvil cell is that measurements in which wires are brought into the high pressure zone, such as electrical resistivity, Hall effect or thermopower, are extraordinarily difficult if a fluid pressure medium is used. As a result, such measurements are normally carried out using solid pressure media which, unfortunately, subject the sample to significant shear stresses. **Rafael Jaramillo** and co-workers at the APS[109] have recently developed a diamond anvil cell for resistivity measurements which uses a methanol-ethanol mixture as fluid pressure medium; this technology has been applied to a detailed study of the suppression of magnetism in pure Cr metal by hydrostatic pressure to 10 GPa. **Isaiah Lim** at **Washington University** has used this new technique to study the effect of hydrostatic pressure on the resistivity of a test sample (Pb) to 4.5 GPa. This cell is shown in Fig. 79. Further experimentation will be necessary before this cell can be used routinely as a diagnostic tool, but the prospects for cleaner magnetic property data at high pressures are promising.

Reflectance of Gold at High Pressure – Temperature measurements in dynamic studies are typically accomplished with streaked visible pyrometry; shocked samples often reach thousands to tens of thousands of degrees and emit copious amounts of Planck radiation. The development of ramp compression methods has led to the ability to quasi-isentropically compress materials; with this load path, temperatures are typically too low to measure with conventional streaked pyrometry. An alternative method, based on the thermoreflectance of gold, is being evaluated in a collaborative effort between **Chris Seagle** and **Dan Dolan** from **SNL** and **Nenad Velisavljevic** from **LANL**.

The spectral reflectance of gold changes dramatically in the visible – hence the characteristic color of gold. The position of the steepest slope in the reflectivity spectrum, and the relative magnitude of the reflectivity in the red and blue regions, are found to be strong functions of temperature suggesting the possibility of a temperature diagnostic for ramp compression studies based on the reflectance of an embedded gold gauge. In order to calibrate a temperature gauge based on the reflectance of gold for dynamic experiments, the pressure and temperature dependence of the reflectivity must be accurately known. A series of isothermal compression measurements on

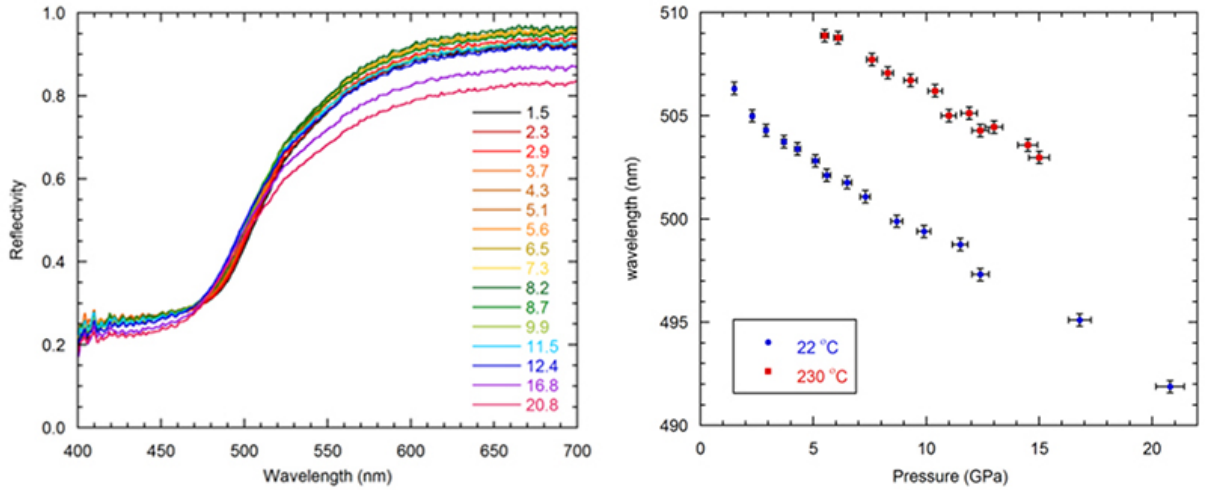


Figure 80. *Left: Visible reflectivity of gold at 22°C. Pressure in GPa is indicated on the right. Right: Position of the steepest slope of the visible reflectivity of gold along two isotherms.*

quantitative reflectivity of gold have been carried out at the **HPCAT** facility and at **SNL**. Figure 80 (left) shows the reflectivity of gold in the visible region upon compression at room temperature. The wavelength of steepest slope is known to be correlated well with temperature; pressure also clearly affects the wavelength of this position. Figure 80 (right) shows the wavelength of this point along the room temperature isotherm and the 230 °C isotherm. Data collection and analysis is ongoing, but Fig. 80 (right) indicates that cross derivatives of the reflectivity with respect to pressure and temperature (*i.e.* $\partial^2 R/\partial P \partial T$) are likely to be small – greatly simplifying a calibration and utilization of the 'gold standard.'

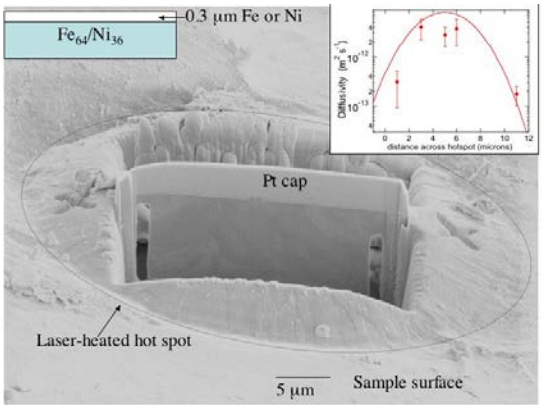


Figure 81. *SEM image of Fe64/Ni36 foil with an initial discontinuity in composition (inset, top left) formed through UHV sputtering after heating to 2200 (±150) K (peak central temperature) at 80 GPa for 3 minutes. SEM image is just before extraction of a TEM foil thinned by focused ion beam milling. EDS profiles from top to bottom as a function of distance across the hotspot show the diffusion of Ni into Fe/Ni alloy (top right). The Pt cap is deposited after extraction from the diamond cell, and provides protection to the top surface of the sample during the milling process.*

Microfabrication of Controlled Geometry Samples – To model and predict material properties under extreme conditions requires accurate and precise measurements of thermoelastic properties. The laser heated DAC coupled with synchrotron-based XRD is a powerful tool to explore pressure-volume-temperature relationships, phase stabilities, and melting curves of materials. The accuracy of measurements of thermoelastic properties such as thermal expansion are hampered by the uncertainty of alignment of the laser-heated spot to the x-ray beam.

Nano- and micro-fabrication techniques (Fig. 81) are used in the **Panero** group at **Ohio State** to create controlled geometry samples with an initial sharp compositional boundary for diffusion and melt determination. *Ex situ* focused ion-beam milling of the sample through the center of a laser-heated spot allows access to information on compositional mixing and diffusion as a function of the distance across the hotspot.

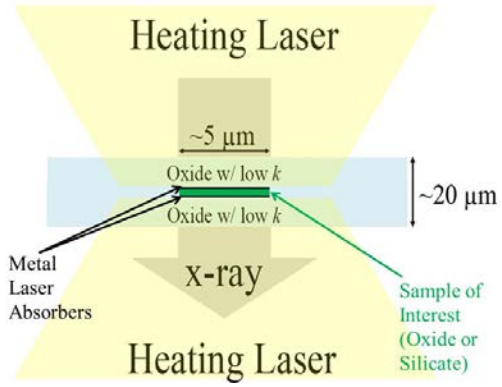


Figure 82. *Sample design of autoaligning samples, with a lateral dimension tuned to the x-ray spot size, and synthesized such that only the sample will absorb the laser.*

Double-sided laser heating of thin samples loaded with thick insulation layers helps reduce axial temperature gradients (Fig. 82). High-pressure, high-temperature EOS parameters also suffer from systematically overestimated temperatures resulting from variations in colinearity of the x-ray beam and the laser-heated spot.[110-112] A controlled geometry sample assures that the heated sample is the hottest portion of the sample. Definitive collinearity will reduce axial temperature gradients and ensure that the diffracting volume is at the peak hotspot temperature. Only the metal portion of the sample can absorb the laser, such that this will be the hottest portion of the sample. If diffraction of the metal is observed, then the diffraction must be from the hottest portion of the sample. This design has been verified by initial experiments on a simplified geometry and the initial steps of producing $>10^6$ such samples as a batch are underway.

4.4 CVD Diamond Research Activities at Carnegie

In this section, we highlight recent principal developments in research on and using chemical vapor deposition (CVD) diamond at Carnegie. While not funded directly by CDAC, the activities of

the CVD diamond group are an integral part of the high pressure group at Carnegie, with several CDAC scientists benefitting from access to anvils fabricated from the CVD diamond material grown at Carnegie. The major achievements have been achieving the largest documented colorless 2.3-carat round diamond, the growth of ultrapure diamond, and the commissioning of the CIW homemade MPCVD reactor with high energetic plasma. The CVD diamond team has provided diamond crystals to numerous research groups around the world. The Carnegie high-pressure group, including CDAC Research Scientists **Maddury Somayazulu** and **Chang-sheng Zha**, obtained the majority of those diamonds. The group has been working closely with high-pressure researchers to gradually improve the performance of various types of CVD diamonds in high-pressure anvil cells. Carnegie Research Scientist **Chih-shiue Yan** coordinates the activities of the CVD team.

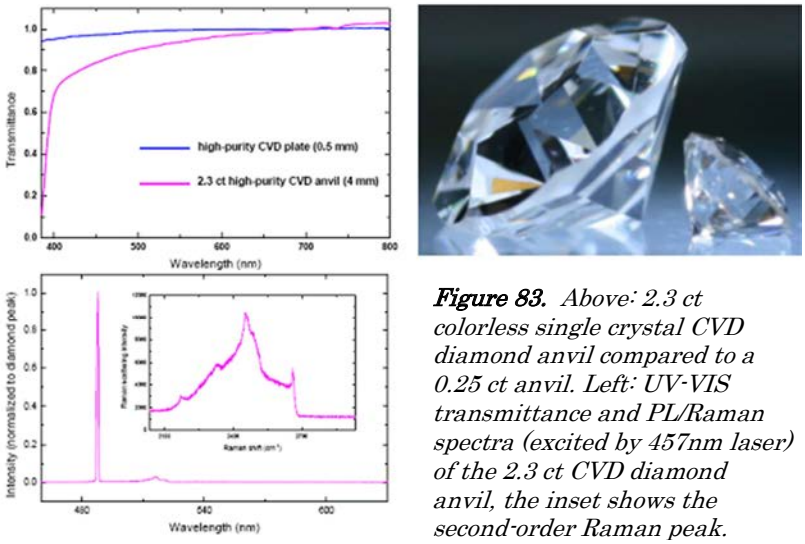


Figure 83. *Above: 2.3 ct colorless single crystal CVD diamond anvil compared to a 0.25 ct anvil. Left: UV-VIS transmittance and PL/Raman spectra (excited by 457nm laser) of the 2.3 ct CVD diamond anvil, the inset shows the second-order Raman peak.*

Large, High-Purity Diamond – Carnegie Research Scientist **Yufei Meng** focuses on the defects in different diamonds and their influence on properties and formation. She has united micro-spectroscopy with high-resolution microscopy to study the point defects and line/face defects and coloration mechanism in brown diamond. The applied spectroscopy methods include PL, FTIR, and EPR. She has obtained monochromatic, high-resolution topographic images of diamonds for the first time using synchrotron radiation. The results give a closer look at the nature of the plastic deformation in brown diamonds. Her recent work includes investigating the growth process, annealing process and characterization of single-crystal diamond grown by MPCVD techniques. This research is aimed at growing large and high-purity single-crystal diamond, in order to further the variety of applications in high-pressure anvils, optical and dielectric windows, monochromators, superhard materials and coatings, semiconductors, quantum materials and other electronic devices.

High-purity CVD single crystal material is technically more difficult to grow than brown material. Finding ways to routinely and reliably produce larger, near-colorless and colorless single-crystal diamond needed for a variety of applications in science and technology is a major challenge. MPCVD techniques have been refined to produce large, high-purity single crystal diamond anvils. Specifically, multicarat single crystal diamond has been produced at a high growth rate without annealing (around 50μm/h) with low impurity content.

The example of a 2.3 carat colorless anvil shown in Fig.83 was cut from a 13.5 carat SC-CVD diamond block grown at high growth rate (around 50 μm/h) in the absence of impurities other than hydrogen. UV-visible absorption, Raman/photoluminescence spectra, cathodoluminescene, and confocal Raman imaging are used to characterize the diamond. The measurements show that the material has high optical quality and clarity without layers. The large intensity ratio of the second-order Raman peak to the fluorescence background (Fig. 83, right) is essential for high-pressure optical windows. PL & CL measurements along growth directions indicate the residual color may be due to an unintentional leak of nitrogen.

Electronic Grade Diamond – High-purity diamond with comparable quality to that of electronic grade diamond from Element 6 (E6) has been achieved at Carnegie. This material has important applications in quantum computing and Raman lasers. This new diamond from an

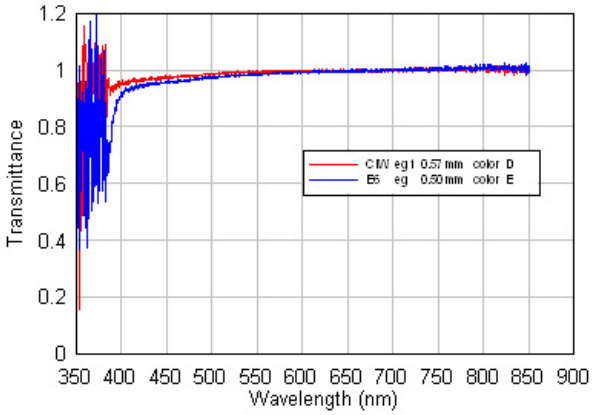


Figure 84. *UV-VIS transmission of CIW eg1 & E6*

enhanced growth process shows comparable PL spectra to the E6 diamond. PL of the new diamond, however, shows a flat and much lower baseline without NV centers and nitrogen aggregates compared with the best diamonds grown before. The new diamond shows a much lower intensity for the Si-V peak than before.

In recent work, two pure CVD diamond plates (samples CIW eg1 & eg2) were fabricated at Carnegie. They were cut into the same size ($4 \times 4 \times 0.5$ mm^3) as an electronic grade CVD diamond from E6 for better comparison. All three samples were characterized by UV-VIS absorption, PL and Raman at room temperature and liquid helium temperature, and by EPR measurements.

Sample CIW eg1 shows obviously higher transmittance than the E6 sample (Fig. 84). E6's lower transmittance below 400 nm may be caused by the absorption of nitrogen. In the absorbance spectra measured with another spectrometer, CIW eg1 also shows lower absorption than the E6 sample within the range from 236 to 1000 nm.

The three samples show comparable PL spectra at room temperature (Fig. 85). NV centers and the Si-V peak are invisible in both CIW eg1 and E6 samples. CIW eg1 has a lower baseline than E6. The intensity ratio of the fluorescence background to the second-order Raman peak (F/R) of CIW eg1 is smaller (0.032) than that of E6 (0.039), which suggests better quality. It may be 10 times better than the good natural diamond anvils (this needs to be confirmed, however). Cooling the samples to 10 K with liquid helium and using longer collecting times, PL of E6 shows an evident NV^- peak at 637 nm, which is invisible in CIW samples. However CIW eg2 has a Si-V peak at 738 nm, which is readily controlled. By using the highest grating and longer collecting time, Raman spectra at 10 K reveal a stronger NV^0 peak at 575 nm in E6 than in the CIW sample. EPR measurements show that the Carnegie diamond is as pure as the E6 electronic grade diamond. The concentration of substitutional nitrogen is below 2 ppb.

Figure 85. *Room temperature PL of CIW eg1, CIW eg2 & E6.*

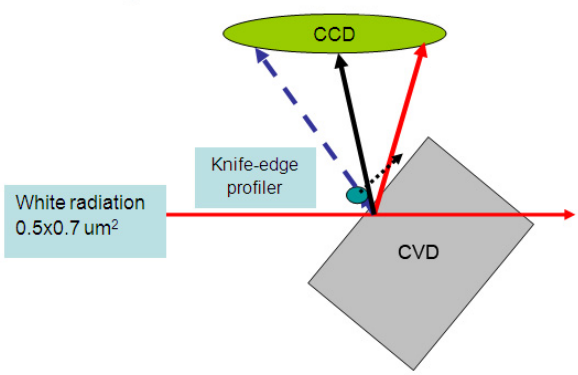


Figure 86. *The schematic of experimental setup.*

X-ray Imaging – CVD diamond can be grown to have hardness equal to, if not superior to, the best natural diamond. In addition, the fracture toughness can be tuned over a very broad range and can be made significantly higher than any natural material. This high toughness will be useful for many applications. To understand the origin of the toughness, we have applied 3-D micro-diffraction techniques to investigate the local lattice rotation and residual strain with 1-micron cube voxel.

Beamline 34IDE at the APS was used for imaging studies. With a differential-aperture x-

ray microscopy technique, it was possible to get a depth resolution of 1 micron along the x-ray beam pass. The typical incident beam size is around 0.5 x 0.7 μm^2. By scanning a knife-edge wire above the sample, and taking the difference of the adjacent white beam Laue diffraction patterns, one can sort the diffraction information from each depth along the incident beam at micron resolution. The schematic of the experimental setup is shown in Fig. 86. An area of 50 x 8 μm^2 was measured. The reconstructed Laue patterns were then analyzed to obtain the local lattice orientation and strain tensors.

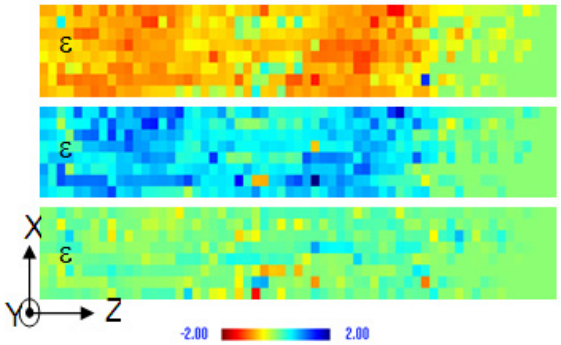


Figure 87 *The local lattice strain maps. The scalar bar is with unit 10^{-3}. X,Y directions are in the sample surface plane, Z is the surface normal direction. There is almost no strain in the normal direction. XYstrain level is up to $2x10^{-3}$.*

The three major components (ε_{xx}, ε_{yy}, ε_{zz}) of the strain tensor at each measured location are displayed in Fig. 87. The strain level is within ± 2 × 10^{-3}. One can see that the strain in ε_{xx} is mostly negative, while ε_{yy} is mostly positive, and ε_{zz} is nearly strain free. There exist two high strain bands in both ε_{xx} and ε_{yy} maps, which indicate the existence of large local strains. The inhomogeneity of strain distribution indicates the local defect arrangement. As each dislocation will induce the lattice rotation, a concept known as the geometrically necessary dislocation (GND) density has been introduced to describe the orientation gradient. Considering the total of 36 slip systems in the face-centered-cubic structure, the <110>{111} type dislocation is dominant. All possible combinations of these 36 slip systems have been analyzed to accommodate the lattice rotation and minimize the total GND density. A simplex method was utilized to achieve the GND density for the area measured. The density calculated is based on the orientation change in the 2-D plane only. The real densities should be higher than those shown due to the lack of orientation gradient in the third direction.

X-ray Topography — A collaboration between the CVD team at Carnegie **(Qi Liang, Chih-shiue Yan, Felix Krasnicki)** and **HPCAT (Dmitry Popov/Changyong Park)** has created the opportunity to study the growth mechanism of single crystal CVD diamond at **HPCAT**. The white beam topography technique was used to evaluate some as-grown CVD single crystal diamonds. CVD single crystals were positioned in the beam at 16-BM-B with the growth axes parallel and/or normal to the beam direction and irradiated with the full spectrum of synchrotron radiation. Multiple x-ray topographs corresponding to reflections from different crystallographic planes were recorded on an x-ray film placed behind the sample at a distance of about 20 cm. Due to the high collimation of the synchrotron radiation, high-resolution images of defects present in the crystal could be produced. An example of the type of image obtained is shown in Fig. 88. Comprehensive studies were performed on different diamond samples: natural, high *P-T* annealed, low pressure-high temperature annealed, as grown with high nitrogen content, as grown colorless, and as grown near colorless diamond. Analysis of the data from these experiments is ongoing.

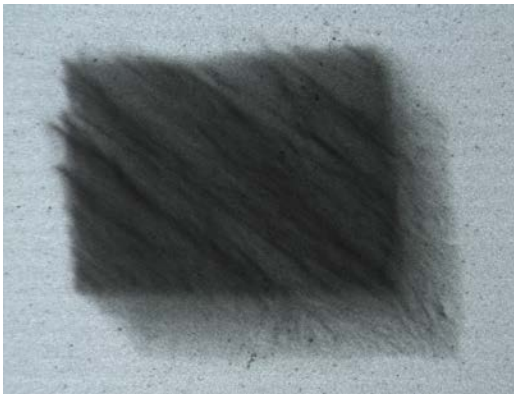


Figure 88. *Example of an x-ray topograph corresponding to a single reflection. It was taken at APS and extracted from an complex white beam topograph of an CVD single crystal.*

Optical Emission Spectra Analysis of Diamond Growth Chemistry — As part of the MPCVD reactor optimization work, plasma analysis is conducted in order to study plasma properties and behavior during diamond growth. A key aspect of single crystal diamond growth via MPCVD is in-process control of the local plasma-substrate environment; *i.e.*, plasma gas phase concentrations of activated species on the plasma

boundary layer near the substrate surface. Optical emission spectra (OES) of the microwave plasma with respect to diamond substrate position inside the microwave plasma reactor chamber have been analyzed. Radical species such as CH, C_2, and H (Balmer series) and their intensities that are important to diamond growth have been identified. The emission intensities of these electronically excited species were found to be more dependent on operating pressure than on microwave power. Also, plasma gas temperatures were measured and calculated using the C_2 Swan band ($d^3\Pi$ $a^3\Pi$ transition) system. The plasma gas temperature ranges from 2800 to 3400 K depending on the spatial location of the plasma ball, microwave power and operating pressure.

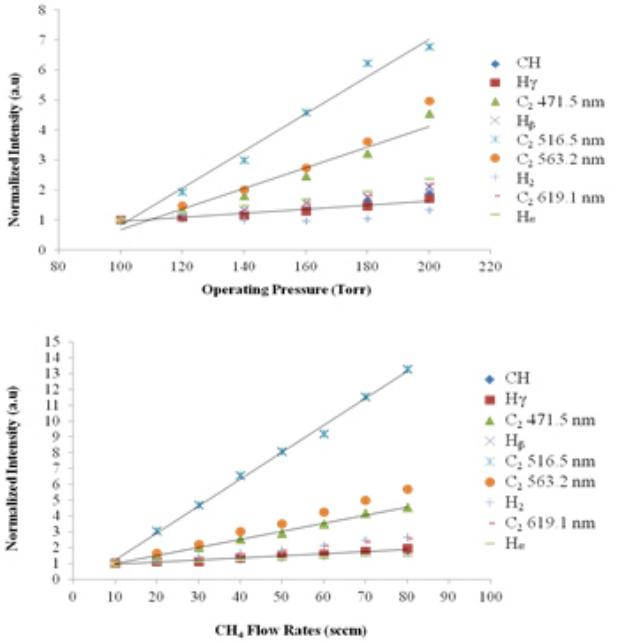


Figure 89. *Top: Normalized emission intensities of CH, Hα, Hβ, Hγ, H_2, and C_2 versus operating pressure. Bottom: Normalized emission intensities of CH, Hα, Hβ, Hγ, H_2, and C_2 versus CH_4 flow rates.*

The normalized intensity of detected species as function of pressure is shown in Fig. 89 (top). As pressure is increased from 100 to 200 Torr, intensities of excited species tend to increase. At 200 Torr, the C_2 intensity of the three peaks (471.5, 516.5, and 563.2 nm) increases to 4.5 to 7 in relative magnitude compared to CH, Hα, Hβ, Hγ, H_2, and CH intensities. This suggests that C_2 is becoming dominant and an important carbon growth species at higher pressure. This is also indicated by the strong visible greenish appearance of the plasma in the reactor chamber during diamond growth. The intensity of Hα increases by a factor of two when the pressure is increased from 100 to 200 Torr. Figure 89 (bottom) shows the normalized intensity of excited species as a function of CH_4 flow rates. C_2 intensity increases significantly as methane flow rates are increased from 10 to 80 sccm. There is a slight "jump" for Hα, Hβ, Hγ, H_2 intensities with increasing CH_4 flow rates, which might indicate an enhancement of plasma electron density.

In another series of experiments, it was found that the C_2 intensity increases when the CH_4 flow rate is increased. However, with the addition of microwave input power from 3250 to 4500 W, the emission intensity of C_2 does not increase significantly. It tends to stay constant for 10 sccm flow rate and slightly increases for 30 and 60 sccm at low power levels but then saturates at higher power levels. The rise in C_2 intensity is much more pronounced with increasing operating pressure than with an increase in microwave input power. This suggests that the C_2 concentration does not depend strongly on microwave input power.

It was observed that, by increasing operating pressure during diamond synthesis, the plasma ball location with respect to substrate position could be highly sensitive. Hence, emission intensities of the dominant excited species were investigated axially and radially. The normalized intensities along the edge of the plasma are essentially constant at around 1, while at the center of the plasma they drop to 0.7. This small drop is due to the increase in Hα emission. This might indicate that there is a higher hydrogen atom concentration at the center of the plasma than at the edge, while the C_2 concentrations are constant across the substrate.

In summary, the increase in C_2 intensity is much more pronounced with increasing operating pressure as compared to an increase in microwave input power. Near the substrate, gas temperature is consistently lower across the substrate at around 2800 K while the calculated gas temperature in the plasma core region is at around 3400 K.

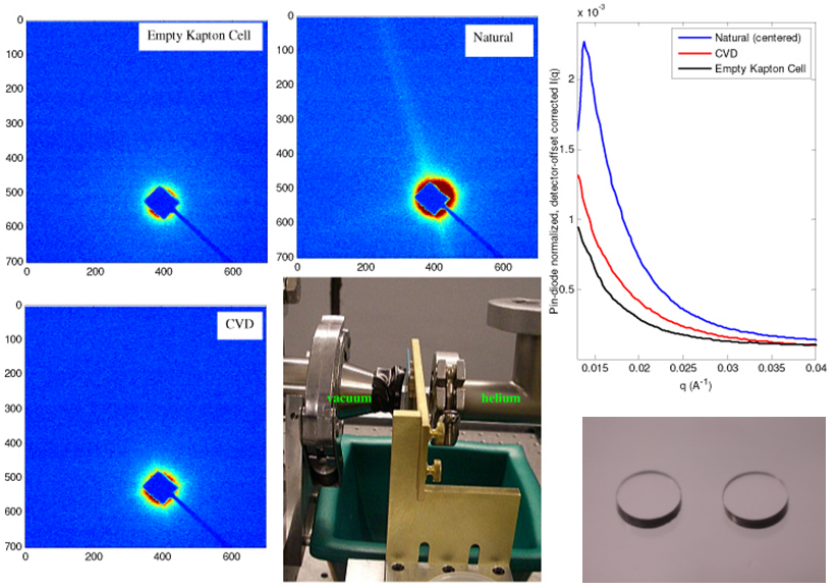


***Figure 90.**. SAXS of an empty Kapton cell, a CVD diamond and a natural diamond with CCD images and setup. The natural diamond shows cross-shaped scattering. The CVD diamond does not show strong cross-shaped scattering. Bottom right: Single-crystal CVD diamond windows for SAXS with 3.0 mm diameter and 0.5 mm thickness.*

Small-Angle X-ray Scattering Windows – Collaborative research with the physics department at Cornell University has shown that the lack of strong cross-shaped scattering (Fig. 90) and the large range of possible dimensions makes CVD diamond promising for small-angle x-ray scattering (SAXS) windows. SAXS was performed on single-crystal CVD diamonds with low nitrogen concentrations, which were fabricated by the MPCVD process at high growth rates. High optical quality, undoped, 500 µm-thick single-crystal CVD diamonds grown without intentional nitrogen addition proved to be excellent as windows on SAXS cells, yielding parasitic scattering no more intense than a 7.5 µm-thick Kapton film. SAXS intensity shows a positive correlation with the intensity of nitrogen-related defect centers in PL. CVD diamond with more nitrogen has stronger SAXS scattering. A single-crystal CVD diamond window has been successfully used in a high-pressure SAXS cell (Fig. 90)

New Diamond-Based Magnetic Sensors – The development of ultra-sensitive induction techniques for magnetic measurements in the diamond cell has allowed measurements on very small samples (down to 20 µm in diameter). However, there is a need to develop more sensitive techniques with much better spatial resolution to observe the details of superconducting and magnetic transitions under high pressure. Recent progress in magnetic sensing from single spins in NV- (nitrogen-vacancy) centers in diamond provides a natural way to monitor the strength of a magnetic field (with nT sensitivity) with the best possible spatial resolution (submicron, and down to nanometer scale) in specially prepared diamond platelets, or in nanodiamonds. A collaboration has recently been established with the Quantum Optics group at the University of Melbourne (led by Professor Steven Prawer) and the Institute of Quantum Optics in Ulm (Director Fedor Jelezko), combining their experience in handling NV- centers, and the high-pressure expertise at Carnegie. We have been able to detect optically the paramagnetic resonance on NV- centers up to 60 GPa, which allows a determination of the pressure shift for the resonance and to measure the magnetic fields using the splitting of the resonance line with the sensitivity of 0.1 mT or better. This is sufficient for detecting a superconducting transition in the typical high-pressure experiment. We are working towards the goal of picking up the resonance from nanodiamonds under pressure, which will allow studies of magnetic properties with unprecedented spatial resolution in a DAC, and embedding NV centers into diamond anvils.

Optically detected magnetic resonance (ODMR) experiments have been performed in a DAC having very small working distance (4.5 mm), which allows the use of standard microbjectives of high quality and with high spatial resolution. The resonance has been measured in two different pressure media: quasihydrostatic NaCl and hydrostatic Ne. The ODMR excitation was achieved by pumping a microwave current into a Pt wire in proximity to the sample in an NaCl medium (Fig 102), embedded into insulating BN+epoxy gasket. In a second experiment with Ne as the pressure medium and a metallic Re gasket, the excitation was achieved by pumping microwave current into a

small copper coil wound around one of the diamond culets. Higher microwave power was pumped in the second case into the coils, and it was possible to detect the ODMR signal reliably, but with a smaller contrast (0.5-2%) than in the case of the Pt wire located in the vicinity of the sample. The pressure has been measured *in situ* from the fluorescence of a small ruby chip located in the DAC, and a standard pressure calibration was applied. A zero-phonon line of NV^- fluorescence was also measured and is shown in Fig. 91, along with the ODMR signal recorded in the NaCl pressure medium. The pressure dependence of the zero-phonon line extrapolates to the excitation wavelength (532 nm) immediately above 60 GPa.

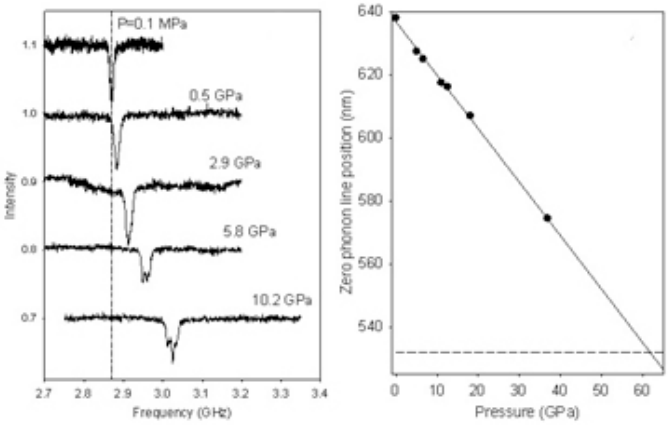


Figure 91. *Left: ODMR in a diamond anvil cell, sample in the NaCl pressure medium. The dashed line is a guide to the eye, indicating the position of the resonance at ambient pressure. Bottom: The pressure shift of the zero phonon line of the fluorescence of NV- centers. Solid line is a linear fit extrapolated to the position of the exciting laser line (532 nm).*

CVD Diamond Growth Facilities at Carnegie — The CVD facilities at Carnegie include five microwave plasma chemical vapor deposition (MPCVD) systems, two laser sawing systems, and two iron wheel polishing machines.

MPCVD #1, Seki AX5500 2.45 GHz 0-10 kW: testing of higher microwave power (5-10 kw) and modification of stages.

MPCVD #2, Seki Ax5500 2.45 GHz 5 kW: production of high purity diamond.

MPCVD #3, Seki AX6500 2.45 GHz, 15 kW: production of large seeds.

MPCVD #4, Seki AX6600950 MHz 75 kW: scaling up diamond synthesis on a large area at rapid growth rate.

MPCVD #5, homemade 2.45 GHz 5 kW: diamond synthesis at rapid growth rate.

In addition, the CVD group uses two sawing lasers (Bettonville Ultrashape II) for sawing and shaping CVD diamonds, and two iron polishing wheels for polishing CVD material.

5. MANAGEMENT AND OVERSIGHT

CDAC has a very horizontal management structure based at **Carnegie**. Active participation by oversight committees assists the management team and allows the maximum amount of resources to be allocated to our three main areas of focus for the Center.

5.1 CDAC Organization and Staff

CDAC is managed at Carnegie by a core staff comprised of the Director, Associate Director, Coordinator, Administrative Assistant and two Laboratory Managers (Fig. 92) Day-to-day operations of the Center are handled by the Director, Coordinator and Assistant, while CDAC laboratory facilities at Carnegie are supervised by the Laboratory Managers.

Russell Hemley, Director, is also a staff scientist and the Director of the Geophysical Laboratory at **Carnegie.** Other members of the Scientific Staff at **Carnegie** that are involved directly with CDAC are:

- **Ronald Cohen** Computational Theory
- **Yingwei Fei** Geochemistry, Petrology and Materials Science
- **Alexander Goncharov** Optical Spectroscopy

- **Timothy Strobel** Energy Materials
- **Viktor Struzhkin** Electronic, Magnetic, and Structural Properties
- **Takamitsu Yamanaka** Senior Visiting Fellow

CDAC staff at **Carnegie** directly supported by the CDAC grant and **Carnegie** Institution matching funds (*i.e.*, indirect cost return) are:

- **Stephen Gramsch** CDAC Coordinator/Research Scientist
- **Morgan Phillips Hoople** CDAC Administrator
- **Maddury Somayazulu** Lab Manager/Research Scientist
- **Chang-sheng Zha** Lab Manager/Research Scientist

Research Scientists at **Carnegie** working on CDAC-related projects include:

- **Muhtar Ahart** (Brillouin spectroscopy)
- **Szczesny Krasnicki** (CVD diamond)
- **Kadek Hemawan** (CVD diamond)
- **Qi Liang** (CVD diamond)
- **Yufei Meng** (CVD diamond)
- **Chih-shiue Yan** (CVD diamond)

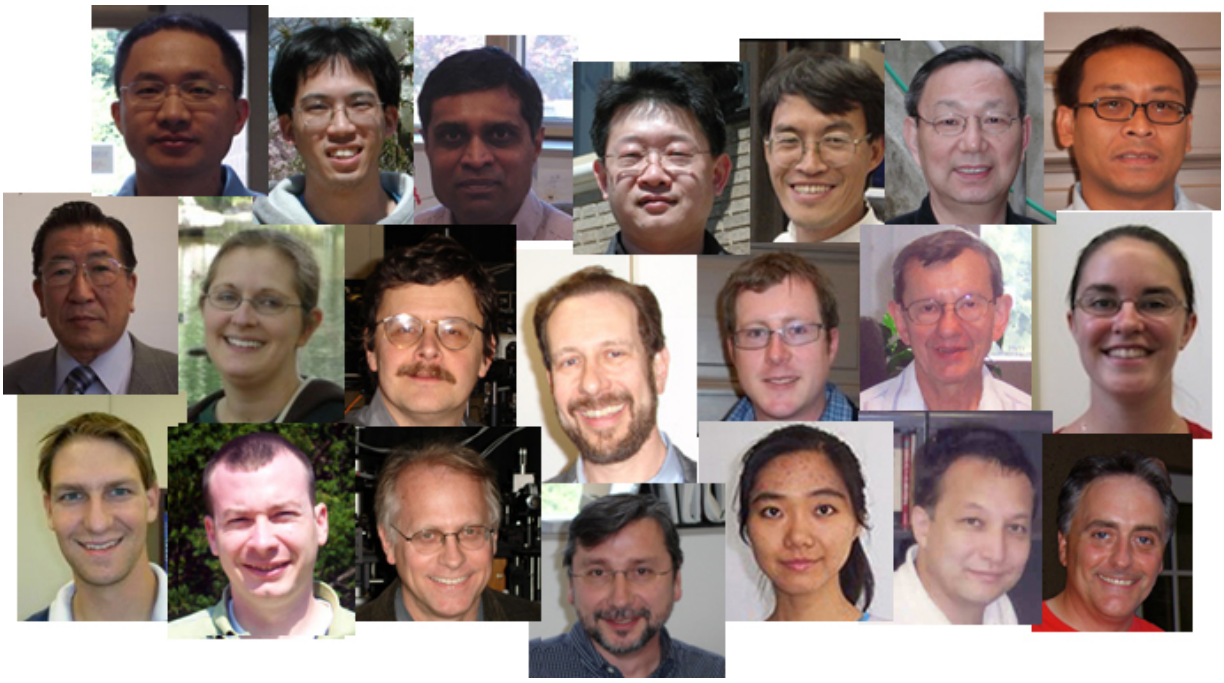


Figure 92. *CDAC affiliated personnel at* ***Carnegie*** *for 2011-2012.*

A number of predoctoral and postdoctoral fellows at **Carnegie** supported by the Institution, other grants, or outside fellowships worked on CDAC tasks during 2011-2012. Their contributions also include training CDAC students, undergraduate summer scholars, and visitors in high-pressure experimental techniques:

- **Caitlin Murphy**
- **Douglas Allen Dalton**
- **Joseph Lai**
- **Stewart McWilliams**

5.2 CDAC Oversight

CDAC Steering and Advisory Committees have been organized to provide guidance to the CDAC research program (Fig. 93). The Steering Committee members informally advise CDAC management on near-term operational issues and act as points of contact with their respective Directorates and Divisions. Steering Committee members also evaluate yearly proposals for graduate student support from the Academic Partners. The CDAC Steering Committee consists of

- **Neal Chesnut** (UWGa)
- **Gilbert W. (Rip) Collins** (LLNL)
- **Dana Dattelbaum** (LANL)
- **Daniel Dolan** (SNL)
- **Jon H. Eggert** (LLNL)
- **David Funk** (LANL)
- **Marcus Knudson** (SNL)
- **Yusheng Zhao** (LANL)
- **Nenad Velisavljevic** (LANL)

The Advisory Committee assists with long-term strategic planning, advises CDAC

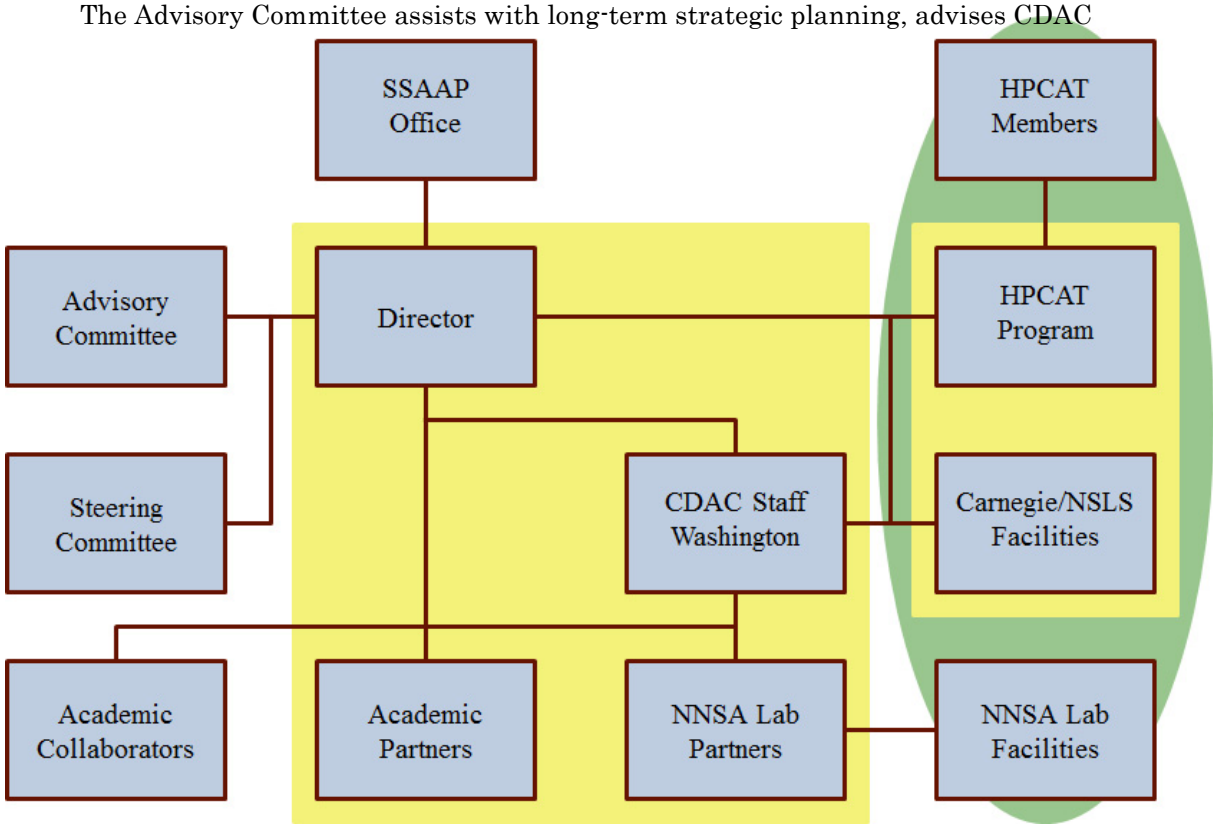


Figure 93. *CDAC organizational chart. The yellow areas designate the principal components of CDAC. The oval area encompasses the three different groups of experimental facilities associated with CDAC.*

management on the scientific program, and provides points of contact between CDAC and the NNSA Labs, other SSAA Centers, and the broader academic community. Current members of the CDAC Advisory Committee are

- **Neil W. Ashcroft** (Cornell)
- **Robert Cauble** (LLNL)
- **Yogendra M. Gupta** (WSU)
- **Alan J. Hurd** (LANL)

- **Chi-chang Kao** (Brookhaven)
- **Christian Mailhiot** (LLNL)
- **Tom Mehlhorn** (SNL)

Members of both CDAC oversight committees are invited to attend regular **HPCAT** meetings and are invited to attend all CDAC functions. Committee members are updated regularly on progress in the scientific program, innovations in technique development, and plans for outreach. Each of the members of the two CDAC committees has agreed to continue serving in their current capacities.

APPENDIX I: CDAC Publications and Presentations for Year 7

We list publications and presentations for 2009-2001, including all work supported fully or in part by CDAC. This list therefore includes work carried out at **HPCAT** by all of its members and users during this period.

A. CDAC Publications

Adams, K. A., S. D. Jacobsen, Z. Liu, S. M. Thomas, M. Somayazulu, and D. M. Jurdy, Optical reflectivity of solid and liquid methane: Application to spectroscopy of Titan's hydrocarbon lakes, *Geophys. Res. Lett.* **39**, L04309 (2012).

Ahart, M., R. E. Cohen, R. J. Hemley, S. Sinogeikin, O. Shebanova, D. Ikuta, and Z. G. Ye, Pressure-dependence of the monoclinic phase in the $Pb(Mg^{1/3}Nb_{2/3})O_3$-$PbTiO_3$ solid solutions, *Phys. Rev. B*, submitted.

Ahart, M., R. E. Cohen, R. J. Hemley, S. V. Sinogeikin, O. Shebanova, D. Ikuta, and Z. G. Ye, Pressure-composition phase diagram of the $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ solid solutions, *Proceedings of The 20th IEEE International Symposium on Applications of Ferroelectrics*, 36-39 (2011).

Ahart, M., C. DeVreugd, J. Li, D. D. Viehland, P. M. Gehring, and R. J. Hemley, X-ray diffraction study of the pressure-induced bcc-to-hcp phase transition in highly magnetostrictive Fe-Ga alloy, *Phys. Rev. B*, submitted.

Ahart, M., M. Somayazulu, S. A. Gramsch, R. Boehler, H. K. Mao, and R. J. Hemley, Brilloun scattering of H_2O-ice to megabar pressures, *J. Chem. Phys.* **134**, 124517 (2011).

Al-Khatatbeh, Y., K. K. M. Lee, and B. Kiefer, Compressibility of nanocrystalline TiO_2 anatase, *J. Phys. Chem. C* **116**, 21635-21639 (2012).

Amin, S., E. N. Rissi, K. McKiernan, and J. L. Yarger, Determining the equation of state of amorphous solids at high pressure using optical microscopy, *Rev. Sci. Instrum.* **83**, 033702 (2012).

Amin, S. A., K. Leinenweber, C. J. Benmore, R. Weber, and J. L. Yarger, Characterizing pressure induced coordination changes in $CaAl_2O_4$ glass using ^{27}Al NMR, *J. Phys. Chem. C* **116**, 2068-2073 (2012).

Andrade, M., D. A. Dzivenko, G. Miehe, R. Boehler, H. T. Hintzen, and R. Riedel, High-pressure high-temperature synthesis and structure of ß-$MgSiN_2$, *Phys. Stat. Solidi RRL* **5**, 196-198 (2011).

Antonangeli, D., T. Komabayashi, F. Occelli, E. Borissenko, A. C. Walters, G. Fiquet, and Y. Fei, SImultaneous sound velocity and density measuremetns of hcp iron up to 93 GPa and 1100 K: An experimental test of the Birch's law at high temperatures, *Earth Planet. Sci. Lett.* **331-332**, 210-214 (2012).

Armentrout, M. M. and A. Kavner, High pressure, high temperature equation of state for Fe_2SiO_4 ringwoodite and implications for the Earth's transition zone, *Geophys. Res. Lett.* **38**, L08309 (2011).

Armstrong, M., J. Crowhurst, A. Goncharov, J. M. Zaug, S. Bastea, and B. Militzer, Shock compression of precompressed deuterium, *AIP Conf. Proc.* **1426**, 791 (2012).

Armstrong, M. R., J. C. Crowhurst, S. Bastea, W. M. Howard, J. M. Zaug, and A. F. Goncharov, Prospects for achieving high dynamic compression with low energy, *Appl. Phys. Lett.* **101**, 101904 (2012).

Armstrong, M. R., J. C. Crowhurst, S. Bastea, J. M. Zaug, and A. F. Goncharov, A path to high density hydrogen with a table top laser, *Nat. Phys.*, submitted.

Bai, L., M. Pravica, Y. Zhao, C. Park, Y. Meng, S. V. Sinogeikin, and G. Shen, Charge transfer in spinel Co_3O_4 at high pressures, *J. Phys.: Cond. Matt.* **24**, 435401 (2012).

Baldini, M., L. Capogna, M. Capone, E. Arcangelitti, C. Petrillo, I. N. Goncharenko, and P. Postorino, Pressure induced magnetic phase separation in $La_{0.75}Ca_{0.25}MnO_3$ magnatite, *J. Phys.: Cond. Matt.* **24**, 045601 (2012).

Baldini, M., Y. Ding, S. Wang, Y. Lin, C. A. Tulk, A. M. Dos Santos, J. F. Mitchell, D. Haskel, and W. L. Mao, Pressure-induced tuning of a magnetic phase separation in $Nd_{0.53}Sr_{0.47}MnO_3$, *Phys. Rev. B* **86**, 094407 (2012).

Baldini, M., V. V. Struzhkin, A. F. Goncharov, P. Postorino, and W. L. Mao, Persistence of Jahn Teller distortion in high pressure metallic phase of $LaMnO_3$, *Phys. Rev. Lett.* **106**, 066402 (2011).

Baldini, M., W. Wang, G. Aquilanti, L. Zhang, Y. Ding, S. Pascarelli, and W. L. Mao, High pressure EXAFS measurements of crystalline Ge using nano-crystalline diamond anvils, *Phys. Rev. B* **84**, 014111 (2011).

Banks, H. B., W. Bi, L. Sun, G. F. Chen, X. H. Chen, and J. S. Schilling, Dependence of Magnetic Ordering Temperature of Doped and Undoped $EuFe_2As_2$ on Hydrostatic Pressure to 0.8 GPa, *Physica C* **471**, 476 (2011).

Barkley, M. C., R. T. Downs, and H. Yang, Structure of walstromite, $BaCa_2Si_3O_9$, and its relationship to $CaSiO_3$-walstromite and wollastonite-II, *Am. Mineral.* **96**, 797-801 (2011).

Barkley, M. C., H. Yang, S. H. Evans, R. T. Downs, and M. J. Origlieri, Redetermination of despujolsite, $Ca_3Mn^{4+}(SO_4)_2(OH)_6$-$3H_2O$, *Acta Cryst. E* **E67**, i47-i48 (2011).

Belonoshko, A. B., M. Ramzan, H. K. Mao, and R. Ahuja, Ionic conductivity in solid molecular hydrogen, *Nature Phys.*, submitted.

Benjamin, A. S., M. Ahart, S. A. Gramsch, L. L. Stevens, E. B. Orler, D. M. Dattelbaum, and R. J. Hemley, Acoustic properties of Kel F-800 copolymer up to 85 GPa, *J. Appl. Phys.* **137**, 014514 (2012).

Benmore, C. J., E. Soignard, M. Guthrie, S. A. Amin, J. K. R. Weber, K. McKiernan, M. C. Wilding, and J. L. Yarger, High pressure x-ray diffraction measurements on Mg_2SiO_4 glass, *J. Non-Cryst. Solids* **357**, 2632-2636 (2011).

Berg, C., A. Lagutchev, Y. Fu, and D. D. Dlott, Nitro stretch probing of a single molecular layer to monitor shock compression with picosecond time resolution, *AIP Conf. Proc.* **1426**, 1573 (2012).

Berg, C. M., K. E. Brown, R. W. Conner, Y. Fu, H. Fujiwara, A. Lagutchev, W. L. Shaw, X. Zheng, and D. D. Dlott, Experiments Probing Fundamental Mechanisms of Energetic Material Initiation and Ignition, *MRS Online Proceedings Library*, 1405 (2012).

Bi, W., Y. Meng, R. S. Kumar, A. L. Cornelius, W. W. Tipton, R. G. Hennig, Y. Zhang, C. Chen, and J. S. Schilling, Pressure-induced structure transition in europium metal to 92 GPa, *Phys. Rev. B* **83**, 104106 (2011).

Bi, W., N. M. Souza-Neto, D. Haskel, G. Fabbris, E. E. Alp, J. Zhao, R. G. Hennig, M. M. Abd-Elmeguid, Y. Meng, R. W. McCallum, K. Dennis, and J. S. Schilling, Synchrotron x-ray spectroscopy studies of valence and magnetic state in europium metal to extreme pressures, *Phys. Rev. B* **85**, 205134 (2012).

Bradley, J. A., K. T. Moore, M. J. Lipp, B. A. Mattern, J. I. Pacold, G. T. Seidler, P. Chow, E. Rod, Y. Xiao, and W. J. Evans, 4 f electron delocalization and volume collapse in praseodymium metal, *Phys. Rev. B* **85**, 100102 (2012).

Brown, K. E., New technologies for spectroscopy of materials under static and shock compression, *Ph.D. Thesis, University of Illinois at Urbana-Champaign* (2012).

Brown, K. E., R. Conner, Y. Fu, and H. Fujiwara, Microscopic states of shocked polymers, *AIP Conf. Proc.* **1426**, 1593 (2012).

Brown, K. E., Y. Fu, W. L. Shaw, and D. D. Dlott, Time-resolved emission of dye probes in a shock-compressed polymer: Effects of te nanostructured energy landscape, *J. Appl. Phys.* **112**, 103508 (2012).

Brown, K. E., W. L. Shaw, X. Zheng, and D. D. Dlott, Simplified laser-driven flyer plates for shock compression science, *Rev. Sci. Instrum.* **83**, 103901 (2012).

Brown, K. E., W. L. Shaw, X. Zheng, and D. D. Dlott, Simplified laser-driven flyer plates for shock compression science, *Rev. Sci. Instrum.* **83**, 103901 (2012).

Caracas, R. and R. J. Hemley, Ferroelctric dense ice, *Phys. Rev. Lett.*, submitted.

Catalli, K., S. H. Shim, P. Dera, V. B. Prakapenka, J. Zhao, W. Sturhahn, P. Chow, Y. Xiao, H. Cynn, and W. J. Evans, Effects of the Fe3+ spin transition on the properties of aluminous perovskite - New insights for lower-mantle seismic heterogeneities, *Earth Planet. Sci. Lett.* **310**, 293-302 (2011).

Chellappa, R., D. M. Dattelbaum, S. Sheffield, and D. Robbins, Pressure-induced polymerization in substituted acetylenes, *AIP Conf. Proc.* **1426**, 1421-1424 (2012).

Chen, B., L. Gao, B. Lavina, P. Dera, E. E. Alp, J. Zhao, and J. Li, Magneto-elastic coupling in compressed Fe_7C_3 supports carbon in Earth's inner core, *Geophys. Res. Lett.* **39**, L18301 (2012).

Chen, B., W. P. Hsieh, D. G. Cahill, D. R. Trinkle, and J. Li, Thermal conductivity of compressed H_2O to 22 GPa: A test of the Leibfried-Sclömann equation, *Phys. Rev. B* **83**, 132301 (2011).

Chen, B., K. Lutker, S. V. Raju, J. Yan, J. Kanitpanyacharoen, J. Lei, S. Yang, H. R. Wenk, H. K. Mao, and Q. Williams, Pressure-promoted texturing in nanocrystalline nickle: Probing the lower size limit of dislocation activity, *Science* **338**, 1448-1451 (2012).

Chen, P. N. and H. K. Mao, Novel dense phases of methane, *J. Chem. Phys.*, submitted.

Chen, P. N., C. S. Zha, X. J. Chen, J. Shu, R. J. Hemley, and H. K. Mao, Raman study of phase transitions in compressed methane using moissanite anvil cells, *Phys. Rev. B* **84**, 104110 (2011).

Chen, X. J., F. J. Jia, J. B. Zhang, Z. X. Qin, L. Y. Tang, L. J. Li, Z. A. Xu, J. Liu, V. V. Struzhkin, R. E. Cohen, and H. K. Mao, Pressure tuning of Fermi surface topology of optimally doped $BaFe_{1.9}Ni_{0.1}As_2$, *Phys. Rev. B*, submitted.

Chen, X. J., J. J. Ying, Z. X. Qin, Z. J. Xiang, H. Wu, Q. Z. Huang, T. Muramatsu, X. F. Wang, P. Cheng, X. H. Chen, W. Yang, V. V. Struzhkin, and H. K. Mao, Angular control of superconductivity in an aromatic hydrocarbon, *Nature*, submitted.

Chen, X. J., C. Zhang, Y. Meng, R. Q. Zhang, H. Q. LIn, V. V. Struzhkin, and H. K. Mao, □-tin->Imma->sh phase transition of germanium, *Phys. Rev. Lett.* **106**, 135502 (2011).

Cheng, J. G., J. S. Zhou, J. B. Goodenough, H. D. Zhou, K. Matsubayashi, Y. Uwatoko, P. P. Kong, C. Q. Jin, W. G. Yang, and G. Y. Shen, Pressure effect of the structural transition and suppression of the high-spin state in the triple-layer T'-$La_4Ni_3O_8$, *Phys. Rev. Lett.* **108**, 236403 (2012).

Chidester, B. A. and T. A. Strobel, The ammonia-hydrogen system under pressure, *J. Phys. Chem.* **115**, 10433-10437 (2011).
Corgne, A., L. S. Armstrong, S. Keshav, Y. Fei, W. F. McDonough, W. G. Minarik, and K. Moreno, Trace element partitioning between majoritic garnet and silicate melt at 10-17 GPa: Implications for a deep mantle process, *Lithos* **148**, 128-141 (2012).
Dalton, D. A., R. S. McWilliams, V. V. Struzhkin, A. F. Goncharov, and M. F. Mahmood, Time resolved diagnostics for pulsed laser heating in diamond anvil cells, *Proceedings of the 27th Army Science Conference*, submitted.
Dalton, D. A., M. Somayazulu, A. F. Goncharov, and R. J. Hemley, Static compression of tetramethylammonium borohydride (TMAB), *J. Phys. Chem. A* **115**, 11033-11038 (2011).
Deng, L., C. T. Seagle, Y. Fei, and A. Shahar, High pressure and temperature electrical resistivity of iron and implications for planetary cores, *Geophys. Res. Lett.*, submitted.
Dera, P., B. Lavina, Y. Meng, and V. Prakapenka, Structural and electronic evolution of Cr_2O_3 on compression to 55 GPa, *J. Solid State Chem.* **184**, 3040-3049 (2011).
Dias, R. P., C. S. Yoo, M. Kim, and J. Tse, Insulator-metal transition of highly compressed carbon disulfide, *Phys. Rev. B* **84**, 144104 (2011).
Ding, Y., Z. Cai, Q. Hu, H. Sheng, J. Chang, R. J. Hemley, and W. L. Mao, Nanoscale diffraction imaging of the high-presesure transition in $Fe_{1-x}O$, *Appl. Phys. Lett.* **100**, 041903 (2012).
Ding, Y., Y. C. Tseng, E. Kaneshita, D. Haskel, M. van Veenendaal, J. Mitchell, and H. K. Mao, Loss of long-range ferromagnetic ordering in mangatite ($La_{0.75}Ca_{0.25}MnO_3$) under pressure, *Phys. Rev. Lett.*, submitted.
Dlott, D. D., New developments in physical chemistry of shock compression, *Annu. Rev. Phys. Chem.* **62**, 575-597 (2011).
Dong, H., S. M. Dorfman, Y. C. Chen, H. Wang, J. Wang, J. Qin, and T. S. Duffy, Compressibility and strength of nanocrystalline tungsten boride under compression to 60 GPa, *J. Appl. Phys.* **111**, 123514 (2012).
Dong, Z., K. K. Zhuravlev, S. A. Morin, L. Li, S. Jin, and Y. Song, Pressure-induced structural transformations of ZnO nanowires probed by x-ray diffraction, *J. Phys. Chem. C* **116**, 2102-2107 (2012).
Dorfman, S. M., V. B. Prakapenka, Y. Meng, and T. S. Duffy, Intercomparison of pressure standards (Au, Pt, Mo, MgO, NaCl, and Ne) to 2.5 Mbar, *J. Geophys. Res.* **117**, B08210 (2012).
Dorfman, S. M., S. R. Shieh, Y. Meng, V. B. Prakapenka, and T. Duffy, Syntesis and equation of stat of perovskites in the $(Mg, Fe)_3Al_2Si_3O_{12}$ system to 177 GPa, *Earth Planet. Sci. Lett.* **357-358**, 194-202 (2012).
Dorfman, S. M., S. R. Shieh, Y. Meng, V. B. Prakapenka, and T. S. Duffy, Synthesis and equation of state of perovskites in the $(Mg,Fe)_3Al_2Si_3O_{12}$ system to 163 GPa, *Earth Planet. Sci. Lett.* **357-358**, 194-202 (2012).
Drozd, V., S. Garimella, S. Saxena, J. Chen, and T. Palasyuk, High-pressure Raman and x-ray diffraction study of ß- and γ-polymorphs of aluminum hydride, *J. Phys. Chem. C* **116**, 3808-3816 (2012).
Duzynska, A., R. Hrubiak, V. Drozd, H. Teisseyre, W. Paszkowicz, A. Reszka, A. Kaminska, A. Durygin, S. K. Saxena, J. D. Fidelus, J. Grabis, C. J. Monty, and A. Suchocki, The structural and optical properties of ZnO bulk and nano crystals under high pressure *High Press. Res.*, in press.
Errandonea, D., R. S. Kumar, S. N. Achary, O. Gomis, F. J. Manjon, R. Shukla, and A. K. Tyagi, New high-pressure phase and equation of state of $Ce_2Zr_2O_8$, *J. Appl. Phys.* **111**, 053519 (2012).
Errandonea, D., R. S. Kumar, J. Lopez-Solano, P. Rodriguez-Hernandez, A. Munoz, M. G. Rabie, and R. Saez Puche, Experimental and theoretical study of structural properties and phase transitions in $YAsO_4$ and $YCrO_4$, *Phys. Rev. B* **83**, 134109 (2011).
Errandonea, D., R. S. Kumar, J. Ruiz-Fuertes, A. Segura, and E. Haussiuhl, High-pressure study of substrate material $SeAlMgO_4$, *Phys. Rev. B* **83**, 144104 (2011).
Esler, K., J. Kim, L. Shulenburger, and D. Ceperley, Accelerating quantum Monte Carlo simulations of real materials on GPU clusters, *Comp. Sci. Eng.* **14**, 40-51 (2012).
Freiman, Y. A., A. Grechnev, S. M. Tretyak, A. F. Goncharov, and R. J. Hemley, Equation of state and Raman-active E_{2g} lattice phonon in phases I, II, and III of solid hydrogen and deuterium, *Phys. Rev. B* **86**, 014111 (2012).
Freiman, Y. A., S. M. Tretyak, A. F. Goncharov, H. K. Mao, and R. J. Hemley, Molecular rotation in ρ-H_2, o-D_2, and HD in phase I under pressure, *J. Low Temp. Phys* **37**, 1302-1306 (2011).
Fu, Y., E. A. Friedman, K. E. Brown, and D. D. Dlott, Vibrational spectroscopy of nitroaromatic self-assembled monolayers under extreme conditions, *Chem. Phys. Lett.* **501**, 369-374 (2011).
Fujiwara, H., K. E. Brown, and D. D. Dlott, A thin-film Hugoniot measurement using a laser-driven flyer plate, *AIP Conf. Proc.* **1426**, 382 (2012).

Galley, M., M. Pravica, and Z. Liu, Studies of melamine at high pressure using far- and mid-infrared spectroscopy, *J. Chem. Phys.*, submitted.
Gamaly, E. G., A. Vailionis, V. Mizeikis, W. Yang, A. V. Rode, and S. Juodkazis, Warm dense matter at the bench-top: Fs-laser-induced confined micro-explosion, *J. HEDP* **8**, 13-17 (2012).
Gao, P., Z. Chen, T. A. Tyson, T. Wu, K. H. Ahn, Z. Liu, S. Kim, and S. W. Cheong, High pressure structural stability of multiferroic hexagonal $REMnO_3$, *Phys. Rev. B* **83**, 224113 (2011).
Gatta, G. D., G. J. McIntyre, J. G. Swanson, and S. D. Jacobsen, Minerals in cement chemistry: a single-crystal neutron diffraction and Raman spectroscopic study of thaumasite, $Ca_3Si(OH)_6(CO_3)(SO_4)_{12}H_2O$, *Am. Mineral.* **97**, 1060-1069 (2012).
Gavriliuk, A. G., V. V. Struzhkin, I. S. Lyubutin, S. G. Ovchinnikov, M. Y. Hu, and P. Chow, Reversible insulator-metal transition in $BiFeO_3$ at high pressure, *Phys. Rev. Lett.*, submitted.
Gavriliuk, A. G., I. A. Trojan, and V. V. Struzhkin, Insulator-metal transition in highly compressed NiO, *Phys. Rev. Lett.* **109**, 086402 (2012).
George, L. and S. K. Saxena, Structural stability of metal hydrides, alanates and borohydrides of alkali and alkali- earth elements: A review, *Int. J. Hydrogen Energ.* **35**, 5454-5470 (2011).
Gleason, A. E., B. Chen, and R. Jeanloz, Elasticity and refractive index of B1-phase NaCL at high pressure, *High Press. Res.*, submitted.
Gomis, O., J. A. Sans, R. Lacomba-Perales, D. Errandonea, Y. Meng, J. C. Chervin, and P. A. Polian, Complex high-pressure polymorphism of barium tungstate, *Phys. Rev. B* **86**, 054121 (2012).
Goncharov, A., J. S. Tse, H. Wang, J. Yang, V. V. Struzhkin, R. T. Howie, and E. Gregoryanz, Bonding, structures, and band gap closures of hydrogen at high pressures, *Phys. Rev. Lett.*, submitted.
Goncharov, A. F., Optical spectroscopy in the diamond anvil cell, in *High-Pressure Physics* (ed. J. Loveday), 155-171 (CRC Press, Boca Raton, FL, 2012).
Goncharov, A. F., Raman spectroscopy at high pressure, *Int. J. Spectrosc.* **2012**, 617528 (2012).
Goncharov, A. F., D. A. Dalton, R. S. McWilliams, and M. F. Mahmood, Development of ultrafast spectroscopic techniques to study rapid chemical and physical changes in materials under extreme pressure and temperature conditions, *MRS Proc.* **1405**, DOI:10.1557/opl.2012.1560 (2012).
Goncharov, A. F., R. J. Hemley, and H. K. Mao, Vibron frequencies of solid H_2 and D_2 to 200 GPa and implications for the P-T phase diagram, *J. Chem. Phys.* **134**, 174501 (2011).
Goncharov, A. F. and V. V. Struzhkin, Comment on "Conductive dense hydrogen" by M. I. Eremets and I. A. Trojan, *Nature Mat.*, submitted.
Goncharov, A. F., V. V. Struzhkin, J. A. Montoya, S. Kharlamova, R. Kundargi, J. Siebert, J. Badro, D. Antonageli, F. J. Ryerson, and H. K. Mao, Spin crossover in iron and thermal conductivity in the Earth's lower mantle, *Phys. Earth Planet. Inter.*, submitted.
Goncharov, A. F., N. Subramanian, T. R. Ravindran, M. Somayazulu, V. Prakapenka, and R. J. Hemley, Polymorphism of dense, hot oxygen, *J. Chem. Phys.* **135**, 084512 (2011).
Goncharov, A. F., M. Wong, D. A. Dalton, J. G. O. Ojwang, V. V. Struzhkin, Z. Konôpková, and P. Lazor, Thermal conductivity of argon at high pressures and high temperatures, *J. Appl. Phys.* **111**, 112609 (2012).
Griffin, P. L., A. Kish, A. Steele, and R. J. Hemley, Differential high-pressure survival in stationary phase Escherichia coli MG1655, *High Press. Res.* **31**, 325-333 (2011).
Guillaume, C., E. Gregoryanz, O. Degtyareva, M. I. McMahon, S. Evans, M. Hanfland, M. Guthrie, S. V. Sinogeikin, and H. K. Mao, Cold melting and solid structures of dense lithium, *Nat. Phys.* **7**, 211-214 (2011).
Guo, J., X. J. Chen, J. Dai, C. Zhang, J. Guo, X. Chen, Q. Wu, D. Gu, P. Gao, L. Yang, K. Yang, X. Dai, H. K. Mao, L. Sun, and Z. Zhao, Pressure-driven quantum criticality in an iron-selenide superconductor, *Phys. Rev. Lett.* **108**, 197001 (2012).
Guthrie, M., R. Boehler, C. A. Tulk, A. M. dos Santos, J. J. Molaison, K. Li, and R. J. Hemley, Neutron-diffraction observations of free protons in dense ice, *Nature*, submitted.
Hamlin, J. J., J. R. Jeffries, N. P. Butch, P. Syers, D. A. Zocco, S. T. Weir, Y. K. Vohra, J. Paglione, and M. B. Maple, High pressure transport properties of the topological insulator $BiSe_3$, *J. Phys.: Cond. Matt.* **24**, 035602 (2012).
Han, W. Q., L. Liu, T. K. Sham, and Z. Liu, Structure and luminescence properties of 10-BN sheets, *Nanoscale* **4**, 6951-6954 (2012).
Han, W. Q., H. G. Yu, and Z. Liu, Convert graphene sheets to BN and BN-C sheets via a carbon-substitution-reaction, *Appl. Phys. Lett.* **98**, 203112 (2011).
Haskel, D., G. Fabbris, N. M. Souza-Neto, M. van Veenendaal, G. Shen, A. E. Smith, and M. A. Subramanian, Stability of the ferromagnetic ground state of La_2MnNiO_6 against large compressive stress, *Phys. Rev. B* **84**, 100403 (2011).

Haskel, D., G. Fabbris, M. Zhernenkov, P. P. Kong, C. Q. Jin, G. Cao, and M. Van Veenendaal, Pressure tuning of the spin-orbit coupled ground state in Sr_2IrO_4, *Phys. Rev. Lett.* **109**, 027204 (2012).

Hazen, R. M., R. J. Hemley, and A. J. Mangum, Carbon in Earth's interior: Storage, cycling, and life, *Eos* **93**, 17-18 (2012).

He, Q., X. Liu, L. Deng, Z. Chen, B. Li, and Y. Fei, Solid solutions between lead fluorapatite and lead fluorvanadate apatate: Compressibility determined by using a diamond-anvil cell coupled with synchrotron x-ray diffraction, *Phys. Chem. Minerals* **39**, 219-226 (2012).

Hemawan, K. W., C. S. Yan, Q. Liang, J. Lai, Y. Meng, S. Krasnicki, H. K. Mao, and R. J. Hemley, Hot spot formation in microwave plasma CVD diamond synthesis, *IEEE Trans. Plasma Sci.* **39**, 2790-2791 (2011).

Hemley, R. J., Dense hydrogen, in *High-Pressure Physics* (ed. J. Loveday), 301-323 (CRC Press, Boca Raton, FL, 2012).

Howie, R. T., C. L. Guillaume, T. Scheler, A. F. Goncharov, and E. Gregoryanz, Mixed molecular and atomic phase of dense hydrogen, *Phys. Rev. Lett.* **108**, 125501 (2012).

Hrubiak, R., V. Drozd, A. Karbasi, and S. K. Saxena, High P-T phase transitions and P-V-T equation of state of hafnium, *J. Appl. Phys.* **111**, 112612 (2012).

Hsieh, W. P., M. D. Losego, P. V. Braun, S. Shenogin, P. Keblinski, and D. Cahill, Testing the minimum thermal conductivity model for amorphous polymers using high pressures, *Phys. Rev. B* **83**, 174205 (2011).

Huang, H., Y. Fei, L. Cai, F. Jing, X. Hu, H. Xie, L. Zhang, and Z. Gong, Evidence for an oxygen-depleted liquid outer core of the Earth, *Nature* **479**, 513-516 (2011).

Huang, H., S. Wu, X. Hu, Q. Wang, X. Wang, and Y. Fei, Shock compression of Fe-FeS mixture up to 200 GPa, *Geophys. Res. Lett.*, submitted.

Hummer, D. R. and Y. Fei, Synthesis and crystal chemistry of Fe^{3+}-bearing $(Mg,Fe^{3+})Si,Fe^{3+})O_3$ perovskite, *Am. Mineral.* **97**, 1915-1921 (2012).

Hunter, L., J. Gordon, S. Peck, D. Ang, and J. F. Lin, Using the Earth as a polarized electron source to search for long-range spin-spin interactions, *Science*, in press.

Irifune, T. and R. J. Hemley, New diamond windows into the Earth, *Eos* **93**, 65-66 (2012).

Ivanov, A. V. and K. D. Litasov, Transition zone water cycle and flood basalt volcanism, *Proc. Nat. Acad. Sci.*, submitted.

Jacobsen, M. K., S. V. Sinogeikin, R. S. Kumar, and A. L. Corgne, High pressure transport characteristics Bi_2Te_3, Sb_2Te_3, and $BiSbTe_3$, *J. Phys. Chem. Solids* **73**, 1154-1158 (2012).

Jeffries, J. R., N. P. Butch, H. Cynn, S. R. Saha, K. Kirshenbaum, S. T. Weir, Y. K. Vohra, and J. Paglione, Interplay between magnetism, structure, and strong electron-phonon coupling in binary FeAs under pressure, *Phys. Rev. B* **83**, 134520 (2011).

Jeffries, J. R., N. P. Butch, K. Kirshenbaum, S. R. Saha, G. K. Samudrala, S. T. Weir, Y. K. Vohra, and J. Paglione, Suppression of magnetism and developmetn of superconductivity within the collapsed tetragonal phase of $Ca_{0.67}Sr_{0.33}Fe_2As_2$ under pressure, *Phys. Rev. B* **85**, 184501 (2012).

Jeffries, J. R., A. L. LIma Sharma, P. A. Sharma, C. D. Spataru, K. McCall, J. D. Sugar, S. T. Weir, and Y. K. Vohra, Distinct supercondicting states in the pressure-induced metallic structures of the nominal semimental Bi_4Te_3, *Phys. Rev. B* **84**, 092505 (2011).

Jeffries, J. R., M. E. Manley, M. A. Wall, K. J. M. Blombaum, and A. J. Schwartz, Hidden disorder in the $\alpha \rightarrow \delta$ transformation of Pu-1.9 at % Ga, *Phys. Rev. B* **85**, 224104 (2012).

Jenei, Z., H. P. Liermann, H. Cynn, J. H. P. Klepeis, B. J. Baer, and W. J. Evans, Structural phase transition in vanadium at high pressure and temperature: Influence of nonhydrostatic conditions, *Phys. Rev. B* **83**, 054101 (2011).

Jia, F. J., W. Yang, L. J. Li, Z. A. Xu, and X. J. Chen, Structural properties of $BaFe_{1.8}Ni_{0.2}As_2$ under pressure, *Physica C* **474**, 1-4 (2012).

Jiang, S., J. Liu, X. LI, L. Bai, W. Xiao, Y. Zhang, C. W. Li, Y. Li, and L. Tang, Phase transformation of Ho_2O_3 at high pressure, *J. Appl. Phys.* **110**, 013526 (2011).

Jing, Z., Y. Wang, T. Yu, T. Sakamaki, Y. Kono, and C. Park, Density and sound velocity of iron-sulfur alloying liquids at high pressures and implications to planetary cores, *Proceedings of the 43rd Lunar and Planetary Science Conference* 2813 (2012).

Kaercher, P., S. Speziale, L. Miyagi, W. Kanitpanyacharoen, and H. R. Wenk, Crystallographic preferred orientation in wustite (FeO) through the cubic-to-rhombohedral phase transition, *Phys. Chem. Minerals* **39**, 613-626 (2012).

Kalita, P. E., A. L. Cornelius, K. E. Lipinska, M. W. Lufaso, Z. R. Kann, S. Sinogeikin, O. A. Hemmers, and H. Schneider, New pressure induced phase transitions in mullite-type $Bi_2(Fe_{4-x}Mn_x)O_{10-\square}$ complex oxides, *Int. J. Mat. Res.* **103**, 464-468 (2012).

Kanagaraj, M., S. Arumugam, R. S. Kumar, N. R. Selvan, S. E. Muthu, J. Prakash, G. S. Thakur, H. Yoshino, K. Murata, K. Matsubayashi, Y. Uwatoko, S. V. Sinogeikin, A. Cornelius, A. K. Ganguli, and Y. Zhao, Correlation between superconductivity and structural properties under high pressure of iron pnictide superconductor $Ce_{0.6}Y_{0.4}AsO_{0.8}F_{0.2}$, *Appl. Phys. Lett.* **100**, 052601 (2012).

Kanitpanyacharoen, W., S. Merkel, L. Miyagi, P. Kaercher, C. N. Tome, Y. Wang, and H. R. Wenk, Significance of mechanical twinning in hexagonal metals at high pressure, *Acta Mater.* **60**, 430-442 (2012).

Kantor, I., V. Prakapenka, A. Kantor, P. Dera, A. Kurnosov, S. Sinogeikin, N. Dubrovinskaia, and L. S. Dubrovinsky, BX90: A new diamond anvil cell designed for X-ray diffraction and optical measurements, *Rev. Sci. Instrum.* **83**, 125102 (2012).

Karbasi, A., S. K. Saxena, and R. Hrubiak, The thermodynamics of several elements at high pressure, *CALPHAD* **35**, 72-81 (2011).

Kavner, A., M. M. Armentrout, E. S. G. Rainey, M. Xie, B. E. Weaver, S. H. Tolbert, and R. B. Kaner, Thermoelastic properties of ReB_2 at high pressures and temperatures and comparison with Pt, Os, and Re, *J. Appl. Phys.* **110**, 093518 (2011).

Kavner, A., M. Weinberger, A. Shahar, R. W. Cumberland, J. B. Levine, R. B. Kaner, and S. H. Tolbert, Lattice strain of osmium diboride under high pressure and nonhydrostatic stress, *J. Appl. Phys.* **112**, 013526 (2012).

Kharlamova, S., V. V. Struzhkin, S. V. Sinogeikin, Y. Xiao, P. Chow, S. L. Bud'ko, N. Ni, and P. C. Canfield, Evidnece for strong correlations in Hund's regime from pressure induced spin crossover in the $SrFe_2As_2$, *Phys. Rev. Lett.*, submitted.

Kim, J. H., J. Y. Choi, M. S. Jeong, J. H. Ko, M. Ahart, Y. H. Ko, and K. J. Kim, Development of a high-pressure brillouin spectrometer and its application to an ethylene-vinyl acetate copolymer, *J. Korean Phys. Soc.* **60**, 1419-1423 (2012).

Kim, M. and C. S. Yoo, Highly repulsive interaction in novel inclusion D_2-N_2 compound at high pressure: Raman and x-ray evidence, *J. Chem. Phys* **134**, 044519 (2011).

Kish, A. L., P. L. Griffin, K. L. Rogers, M. L. Fogel, R. J. Hemley, and A. Steele, High-pressure tolerance in Halobacterium salinarum NRC-1 and ohter non-piezophilic prokaryotes, *Extremophiles* **16**, 355-361 (2012).

Kojima, S., M. Ahart, V. Sivasubramanian, A. A. Bokov, and Z. G. Ye, Precursor dynamics of $Pb(B_{1/2}B'_{1/2})O_3$ based relaxor ferroelectrics studied by broadband micro-Brillouin scattering, *J. Adv. Dielect.* **2**, 1241004 (2012).

Kong, L., L. Wang, S. C. Zhang, O. Tschauner, Y. Zhao, W. Yang, H. Liu, and H. K. Mao, In situ structure characterization of $Pb(Yb_{1/2}Nb_{1/2})O_3$-$PbTiO_3$, *Appl. Phys. Lett.* **101**, 062904 (2012).

Kono, Y., C. Kenny-Benson, C. Park, G. Shen, and Y. Wang, Anomaly in the viscosity of liquid KCl at high pressures, *Phys. Rev. B*, in press.

Kono, Y., C. Park, T. Sakamaki, C. Kenny-Benson, G. Shen, and Y. Wang, Simultaneous structure and elastic wave velocity measurements of SiO_2 glass at high pressures and high temperatures in a Paris-Edinburgh cell, *Rev. Sci. Instrum.* **83**, 033905 (2012).

Kono, Y. and Y. Wang, Elastic wave velocity measurement combined with synchrotron x-ray measurements at high pressure and high temperature conditions: Towards prediction and reproduction of MoHole rocks, *Chikyu Monthly* **34**, 211-225 (2012).

Konôpková, Z., P. Lazor, A. F. Goncharov, and V. V. Struzhkin, Thermal conductivity of hcp iron at high pressures and temperatures, *High Press. Res.* **31**, 228-236 (2011).

Kumar, R. S., D. Antonio, M. Kanagaraj, S. Arumugam, A. Cornelius, S. V. Sinogeikin, J. Prakash, G. S. Thakur, A. K. Ganguli, T. Hartmann, and Y. Zhao, Pressure effect on crystal structure and superconductivity of $La_{0.8}Th_{0.2}FeAsO$, *Phys. Stat. Sol. RRL* **5**, 208-210 (2011).

Kumar, R. S., D. Antonio, M. Kanagaraj, S. Arumugam, J. Prakash, S. V. Sinogeikin, G. S. Thakur, A. K. Ganguli, A. L. Cornelius, and Y. Zhao, Pressure induced structural transition and enhancement of superconductivity in Co doped CeFeAsO, *Appl. Phys. Lett.* **98**, 012511 (2011).

Kung, A., A. F. Goncharov, C. S. Zha, P. Eng, and W. L. Mao, Compressional, temporal, and compositional behavior of H_2-O_2 compound formed by high pressure x-ray irradiation, *J. Chem. Phys.* **134**, 234502 (2011).

Kurakevych, O. O., T. A. Strobel, D. Y. Kim, T. Muramatsu, and V. V. Struzhkin, Ni-Si clathrates are high-pressure phases: A melt-based route to conrol stoichiometry and properties, *Crystal Growth Design*, submitted.

Kyono, A., M. Ahart, T. Yamanaka, H. K. Mao, and R. J. Hemley, High-pressure Raman spectroscopic studies of ulvöspinel Fe_2TiO_4, *Am. Mineral.* **96**, 1193-1198 (2011).

Kyono, A., S. A. Gramsch, T. Yamanaka, D. Ikuta, M. Ahart, B. Mysen, H. K. Mao, and R. J. Hemley, The influence of the Jahn-Teller effect at Fe^{2+} on the structure of chromite at high pressure, *Phys. Chem. Minerals* **39**, 131-141 (2012).

Lavina, B., P. Dera, E. Kim, Y. Meng, R. T. Downs, P. F. Weck, S. R. Sutton, and Y. Zhao, Discovery of the recoverable high-pressure iron oxide Fe_4S_5 *Proc. Nat. Acad. Sci.* **108**, 17281-17285 (2011).

Lazicki, A., P. Loubeyre, F. Occelli, R. J. Hemley, and M. Mezouar, Static compression of LiH to 250 GPa, *Phys. Rev. B* **85**, 054103 (2012).

Lebegue, S., C. Moyses Araujo, D. Y. Kim, M. Ramzan, H. K. Mao, and R. Ahuja, Semi-metallic dense hydrogen at 260 GPa, *Proc. Nat. Aca. Sci.* **109**, 9766-9769 (2012).

Lee, S. K., S. Y. Park, H. I. Kim, O. Tschauner, P. Asimow, L. Bai, Y. Xiao, and P. Chow, Structure of shock compressed model basaltic glass: Insights from O K-edge x-ray Raman scattering and high-resolution ^{27}Al NMR spectroscopy, *Geophys. Res. Lett.* **39**, L05306 (2012).

Lee, Y., Y. Lee, D. Suong, J. H. Im, H. J. Hwang, T. H. Kim, D. Liu, Z. Liu, S. Y. Lee, C. C. Kao, and T. Vogt, Immobilization of large, aliovalent cations in the small-pore zeollite k-natrolite by means of pressure, *Angew. Chem. Int. Ed.* **20**, 4932-4935 (2012).

Lee, Y., D. Liu, D. Seoung, Z. Liu, C. C. Kao, and T. Vogt, Pressure- and heat-induced insertion of CO_2 into an auxetic small-pore zeolite, *J. Am. Chem. Soc.* **133**, 1674-1677 (2011).

Li, B., Y. Ding, W. Yang, L. Wang, B. Zou, J. Shu, S. V. Sinogeikin, C. Park, G. Zou, and H. K. Mao, Calcium with the □-tin structure at high pressure and low temperature, *Proc. Nat. Acad. Sci.* **109**, 16459-16462 (2012).

Li, J. and Y. Fei, Experimental constraints on core composition, In Treatise on geochemistry, in *Treatise on Geochemistry* (eds. H. D. Holland and Turekian, K. K.), in press (Elsevier Ltd., Oxford).

Li, S., Q. Li, K. Wang, X. Tan, M. Zhou, B. Li, B. Liu, G. Zou, and B. Zou, Pressure-induced phase transition in guanidinium perchlorate: A supramolecular structure directed by hydrogen bonding and electrostatic interactions, *J. Phys. Chem. B* **115**, 11816-11822 (2011).

Li, S., K. Wang, M. Zhou, Q. Li, B. Liu, G. Zou, and B. Zou, Pressure-induced phase transitions in ammonium squarate: A supramolecular structure based on hydrogen-bonding and □-stacking interactions, *J. Phys. Chem. B* **115**, 8981-8988 (2011).

Li, Y. L., X. J. Chen, Z. Zheng, H. K. Mao, and H. Q. Lin, Density functional calculation of the electronic and lattice properties of solid SnH_4 under pressure: A possible route to a high-temperature superconducting state, *Phys. Rev. Lett.*, submitted.

Li, Z., L. Wang, B. Liu, J. Wang, B. Liu, Q. Li, B. Zou, T. Cui, Y. Meng, H. K. Mao, Z. Liu, and J. Liu, The structural transition behavior of CdSe/ZnS core/shell quantum dots under high pressure, *Phys. Stat. Sol. B* **5**, 1149-1153 (2011).

Lin, D., W. Lei, Z. Liu, and Y. Lee, Spectroscopic study of pressure-induced phase transitions in natrolite, *Phys. Chem. Chem. Phys*, submitted.

Lin, J. F., E. E. Alp, and A. F. Goncharov, Raman and nuclear resonant spectroscopy in geoscience, in *Treatise on Geophysics* **207**, 81-88 (2012).

Lin, J. F., E. E. Alp, Z. Mao, T. Inoue, C. A. McCammon, Y. Xiao, P. Chow, and J. Zhao, Electronic spin states of ferrous iron in the lower-mantle silicate perovskite *Am. Mineral.* **97**, 591-597 (2012).

Lin, J. F., Y. Q. Cai, N. Hiraoka, T. Okuchi, E. Schwegler, Z. Jenei, and W. J. Evans, Dissociation of the high-density water by x-ray irradiation, *J. Chem. Phys.*, submitted.

Lin, J. F., N. Hiraoka, T. Okuchi, Y. Q. Cai, E. Schwegler, and Z. Jenei, X-ray induced dissociation in liquid H_2O at high pressure and temperature, *Phys. Rev. B*, submitted.

Lin, J. F., J. Liu, C. Jacobs, and V. B. Prakapenka, Vibrational and elastic properties of ferromagnesite across the electronic spin-pairing transition of iron, *Am. Mineral.* **97**, 583-591 (2012).

Lin, J. F., J. S. Tse, E. E. Alp, J. Zhao, M. Lerche, W. Sturhahn, Y. Xiao, and P. Chow, Phonon density of states of Fe_2O_3 across high-pressure structural and electronic transitions, *Phys. Rev. B* **84**, 064424 (2011).

Lin, J. F. and A. Wheat, Electronic spin transition of iron in Earth's lower mantle by Mössbauer spectroscopy, *Hyperfine Interact.* **207**, 81-88 (2012).

Lin, Y., H. Ma, C. W. Matthews, B. Kolb, S. Sinogeiken, T. Thonhauser, and W. L. Mao, Experimental and theoretical studies on a high pressure monoclinic phase of ammonia borane, *J. Phys. Chem C* **16**, 2172-2178 (2012).

Lin, Y., Y. Yang, H. Ma, Y. Cui, and W. L. Mao, Compressional behavior of bulk and nanorod $LiMn_2O_4$ under nonhydrostatic stress, *J. Phys. Chem. C* **115**, 9844-9849 (2011).

Lin, Y., L. Zhang, H. K. Mao, P. Chow, Y. Xiao, M. Baldini, J. Shu, and W. L. Mao, Amorphous diamond - A high-pressure superhard carbon allotrope, *Phys. Rev. Lett.* **107**, 175504 (2011).

Lin, Z. J., J. Z. Zhang, B. S. Li, L. P. Wang, H. K. Mao, R. J. Hemley, and Y. Zhao, Superhard diamond/tungsten carbide nanocomposites, *Appl. Phys. Lett.* **98**, 121914 (2011).

Lipp, M. J., A. P. Sorini, J. Bradley, B. Maddox, K. T. Moore, H. Cynn, T. P. Devereaux, Y. Xiao, P. Chow, and W. J. Evans, X-ray emission spectroscopy of cerium across the □-□ volume collapse transition, *Phys. Rev. Lett.* **109**, 195705 (2012).

Litasov, K. D., A. F. Goncharov, and R. J. Hemley, Crossover from melting to dissociation of CO_2 under pressure: Implications for the lower mantle, *Earth Planet. Sci. Lett.* **309**, 318-323 (2011).

Liu, D., Z. Liu, Y. Lee, D. Seoung, and Y. Lee, Spectroscopic characterization of alkali-metal exchanged natrolites, *Am. Mineral.* **97**, 419-424 (2012).

Liu, D., D. Seoung, Y. Lee, Z. Liu, J. W. Lee, J. H. Yoon, and Y. Lee, High-pressure spectroscopic study of hydrous and anhydrous Cs-exchanged natrolites, *J. Phys. Chem.* **116**, 2159-2164 (2012).

Liu, Q. Q., X. Yu, X. Wang, Z. Deng, Y. X. Lv, J. Zhu, S. C. Zhang, H. Liu, W. Yang, L. Wang, H. K. Mao, G. Shen, Z. Lu, Y. Ren, Z. Chen, Z. Lin, and C. Jin, Pressure-induced isostructural phase transition and correlation of FeAs coordination with the superconducting properties of 111-type $Na_{1-x}FeAs$ *J. Alloy Comp.* **133**, 7892-7896 (2011).

Liu, X., J. Chen, J. Tang, Q. He, S. Li, F. Peng, D. He, L. Zhang, and Y. Fei, A large volume cubic press with a pressure-generating capability up to about 10 GPa, *High Press. Res.* **32**, 239-254 (2012).

Liu, X., S. Wang, Q. He, J. L. Chen, H. Wang, S. Li, F. Peng, L. Zhang, and Y. Fei, Thermal elastic behavior of $CaSiO_3$-walstromite: A powder x-ray diffraction study up to 900 C, *Am. Mineral.* **97**, 262-267 (2012).

Lozano, A., Viscosity of water at high pressure and high temperatures, *Masters Thesis, Ohio State University* (2011).

Lucas, M. S., L. Mauger, J. A. Munoz, Y. Xiao, A. O. Sheets, S. L. Semiatin, J. Horwath, and Z. Turgut, Magnetic and vibrational properties of high-entropy alloys, *J. Appl. Phys.* **109**, 07E307 (2011).

Ma, H., B. Liu, Q. Li, X. Zhang, Q. Zeng, S. Yu, B. Zou, T. Cui, G. Zou, Z. Liu, and T. Wagberg, Synchrotron x-ray diffraction and infrared spectroscopy studies of $C_{60}H_{18}$ under high pressure, *ACS Nano*, submitted.

Machida, A., M. Honda, T. Hattori, A. Sano-Furukawa, T. Watanuki, Y. Katayama, K. Aoki, K. Komatsu, H. Arima, H. Ohshita, T. Otomo, M. Tsubota, K. Doi, T. Ichikawa, Y. Kojima, and D. Y. Kim, Formation of NaCl-type monodeuteride LaD by disproportionation reaction of LaD_2, *Phys. Rev. Lett.* **108**, 205501 (2012).

MacLeod, S. G., B. E. Tegner, H. Cynn, W. J. Evans, J. E. Proctor, M. I. McMahon, and G. J. Ackland, Experimental and theoretical study of Ti-6Al-4V to 220 GPa, *Phys. Rev. B* **85**, 224202 (2012).

Mailman, A., S. M. Winter, X. Yu, C. M. Robertson, W. Yong, J. S. Tse, R. A. Secco, Z. Liu, P. A. Dube, J. A. K. Howard, and R. T. Oakley, Crossing the metal-insulator barrier with a thiazol radical conductor, *J. Am. Chem. Soc.* **134**, 9886-9889 (2012).

Mao, H. K., Y. Ding, Y. Xiao, P. Chow, J. Shu, S. Lebegue, A. Lazicki, and R. Ahuja, Electronic dynamics and plasmons of sodium under compression, *Proc. Nat. Acad. Sci.* **108**, 20434-20437 (2011).

Mao, Z., S. M. Dorfman, S. R. Shieh, J. F. Lin, V. Prakapenka, Y. Meng, and T. Duffy, Equation of state of a high-pressure phase of $Gd_3Ga_5O_{12}$, *Phys. Rev. B* **83**, 054114 (2011).

Mao, Z., S. D. Jacobsen, D. J. Frost, C. A. McCammon, E. Hauri, and T. S. Duffy, Effect of hydration on the single-crystal elastic properties of Fe-bearing wadsleyite to 12 GPa, *Am. Mineral.* **96**, 1606-1613 (2011).

Mao, Z., J. F. Lin, A. Alatas, and J. Zhao, Power-law velocity-density behavior of iron in Earth's inner core, *Nat. Geophys.*, submitted.

Mao, Z., J. F. Lin, S. D. Jacobsen, T. S. Duffy, Y. Y. Chang, J. R. Smyth, D. J. Frost, E. H. Hauri, and V. B. Prakapenka, Sound velocities of hydrous ringwoodite to 16 GPa and 673 K, *Earth Planet. Sci. Lett.* **331-332**, 112-119 (2012).

Mao, Z., J. F. Lin, J. Liu, A. Alatas, L. Gao, J. Zhao, and H. K. Mao, Sound velocities of Fe and Fe-Si alloys in the Earth's core, *Proc. Nat. Acad. Sci.* **109**, 10239-10244 (2012).

Mao, Z., J. F. Lin, J. Liu, and V. B. Prakapenka, Thermal equation of state of lower-mantle ferropericlase across the spin crossover, *Geophys. Res. Lett.* **38**, 23 (2011).

Mao, Z., J. F. Lin, H. Scott, H. C. Watson, V. B. Prakapenka, Y. Xiao, P. Chow, and C. A. McCammon, Iron-rich perovskite in the Earth's lower mantle, *Earth Planet Sci. Lett.* **309**, 179-184 (2011).

Marquardt, H., A. E. Gleason, K. Marquardt, S. Speziale, L. Miyagi, G. Neusser, H. R. Wenk, and R. Jeanloz, Elastic properties of nano-crystalline MgO powder to high pressures by Brillouin light scattering, *Phys. Rev. B* **84**, 064131 (2011).

Marques, M., M. Santoro, C. Guillaume, C. Gorelli, J. Contreras-Garcia, A. F. Goncharov, and E. Gregoryanz, On optical properties of dense sodium, *Phys. Rev. Lett.* **83**, 184106 (2011).

McWilliams, R. S., Y. Kadry, M. F. Mahmood, A. F. Goncharov, and J. Ciezak-Jenkins, Structural and chemical properties of the nitrogen-rich energetic material triaminoguanidium 1-methyl-5-nitriminotetrazolate under pressure, *J. Chem. Phys.* **137**, 054501 (2012).

McWilliams, R. S., D. K. Spaulding, J. H. Eggert, P. M. Celliers, D. G. Hicks, R. F. Smith, G. W. Collins, and R. Jeanloz, Phase transformations and metallization of magnesium oxide at high pressure and temperature, *Science* **338**, 1330-1333 (2012).

Mei, Q., G. Shen, V. Prakapenka, P. Lazor, S. V. Sinogeikin, Y. Meng, and C. Park, Helium effect on intermediate range order structure changes in SiO_2 glass under high pressure, *Phys. Rev.*, submitted.

Meng, Y. F., C. S. Yan, S. Krasnicki, Q. Liang, J. Lai, H. Shu, T. Yu, A. S. Steele, H. K. Mao, and R. J. Hemley, High optical quality multicarat single crystal diamond produced by chemical vapor deposition, *Phys. Stat. Sol. (a)* **209**, 101-104 (2012).

Mibe, K., T. Kawamoto, K. N. Matsukage, Y. Fei, and S. Ono, Slab melting versus slab dehydration in subduction-zone magmatism, *Proc. Nat. Acad. Sci.* **108**, 8177-8182 (2011).

Militzer, B., E. L. Pollock, and D. Ceperley, Path integral Monte Carlo calculation of the momentum distribution of the homogeneous electron gas at finite temperature, *Phys. Rev. B*, submitted.

Miyagi, L., W. Kanitpanyacharoen, J. Knight, V. Raju, P. Kaercher, H. R. Wenk, Q. Williams, and E. Zepeda, Combined resistive and laser heating in diamond anvil high pressure experiments, *Rev. Sci. Instrum.*, submitted.

Miyagi, L., W. Kanitpanyacharoen, S. Stackhouse, B. Militzer, and H. R. Wenk, The effect of grain size on Deformation and texture development in $MgGeO_3$ post-perovskite, *Earth Planet. Sci. Lett.*, submitted.

Miyagi, L., W. Kanitpanyacharoen, S. Stackhouse, B. Militzer, and H. R. Wenk, The enigma of post-perovskite anisotropy: Deformation versus transformation textures, *Phys. Chem. Minerals* **38**, 665-678 (2011).

Mizeikis, V., A. Vailionis, E. G. Gamaly, W. Yang, A. Rode, and S. Joudkazis, Synthesis of super-dense phase of aluminum under extreme pressure and temperature conditions created by femtosecond laser pulses in sapphire, *Proc. of SPIE* **8249**, 82490A (2012).

Mohanty, P., B. Kokosza, C. Liu, M. Weinberger, M. Mandal, V. Stagno, Y. Fei, and K. Landskron, Large-pore periodic mesporous silicas with crystalline channel walls and exceptional hydrothermal stability synthesized by a general high-pressure nanocasting route, *Microporous Mesoporous Mater.* **152**, 214-218 (2012).

Mohanty, P., M. Weinberger, Y. Fei, and K. Landskron, Large-pore periodic mesporous quartz, *J. Am. Chem. Soc.*, submitted.

Montgomery, J. M., B. Kiefer, and K. K. M. Lee, Determining the phase transition boundary in highly-ordered pyrolitic graphite with time-dependent resistance measurements, *J. Appl. Phys.* **110**, 047325 (2011).

Montgomery, J. M., G. K. Samudrala, G. M. Tsoi, and Y. K. Vohra, High-pressure phase transitions in rare earth metal thulium to 195 GPa, *J. Phys.: Cond. Matt.* **23**, 155701 (2011).

Montoya, J. A. and A. F. Goncharov, Finite element calculations of the time dependent thermal fluxes in the laser-heated diamond anvil cell, *J. Appl. Phys.* **111**, 112617 (2012).

Munoz, J. A., M. S. Lucas, O. Delaire, M. Winterrose, L. Mauger, C. W. Li, A. O. Sheets, M. B. Stone, D. L. Abernathy, Y. Xiao, P. Chow, and B. Fultz, Positive vibrational entropy of chemical ordering in FeV, *Phys. Rev. Lett.* **107**, 115501 (2011).

Murakami, M., A. F. Goncharov, N. Hirao, R. Masuda, and T. Mitsui, Reduction of radiative thermal conductivity in the deep terrestrial magma ocean, *Nature*, submitted.

Musfeldt, J. L., Z. Liu, S. Li, J. Kang, C. Lee, P. Jena, J. L. Manson, J. A. Schlueter, G. L. Carr, and M. H. Whangobo, Pressure-induced local structure distortions in $Cu(pyz)F_2(H_2O)_2$, *Inorg. Chem.* **50**, 6347-6352 (2011).

Nakamoto, Y., M. Sakata, T. Yamanaka, K. Shimizu, Y. Meng, S. V. Sinogeikin, S. Kharlamova, V. V. Struzhkin, H. K. Mao, and R. J. Hemley, Superconducting T_c of 22 K and crystal structure of yttrium at megabar pressures, *Phys. Rev. Lett.*, submitted.

Niu, H., X. Q. Chen, S. Wang, D. Li, W. L. Mao, and Y. Li, Families of superhard crystalline carbon allotropes constructed via cold compression of graphite and nanotubes, *Phys. Rev. Lett.* **108**, 135501 (2012).

Niu, H., W. Sun, Q. Shan, H. Zhang, X. Chen, Y. Fei, and X. Yu, Deeply subducted oceanic gabbro back to the surface through serpentinite segregation, *Science*, submitted.

Oh, J. E., S. M. Clark, H. R. Wenk, and P. J. M. Monteiro, Experimental determination of bulk modulus of 14A tobermorite using high pressure synchrotron x-ray diffraction, *Cement Concrete Res.* **42**, 397-403 (2012).

Ohta, K., R. E. Cohen, K. Hirose, K. Haule, K. Shimizu, and Y. Ohishi, Experimental and theoretical evidence for pressure-induced metallization in FeO with the rocksalt-type structure, *Phys. Rev. Lett.* **108**, 026403 (2012).

Ojwang, J. G. O., R. S. McWilliams, and A. F. Goncharov, Melting and dissociation of ammonia at high pressure and high temperature, *J. Chem. Phys.* **137**, 064507 (2012).

Okamura, H., N. Ohta, A. Takigawa, I. Matsutori, K. Shoji, K. Miyata, M. Matsunami, H. Sugawara, C. Sekine, I. Shirotani, H. Sato, T. Moriwaki, Y. Ikemoto, Z. Liu, and G. L. Carr, Pressure suppression of

unconventional charge-density-wave state in $PrRu_4P_{12}$ studied by optical conductivity, *Phys. Rev. B* **85**, 205116 (2012).
Pacold, J. I., J. A. Bradley, B. A. Mattern, M. J. Lipp, G. T. Seidler, P. Chow, Y. Xiao, E. Rod, B. Rusthoven, and J. Quintana, A miniature x-ray emission spectrometer (miniXES) for high-pressure studies in a diamond anvil cell, *J. Synchrotron Rad.* **19**, 245-251 (2012).
Panero, W. R., J. R. Smyth, J. S. Pigott, Z. Liu, and D. J. Frost, Hydrous ringwoodite to 5 K and 35 GPa: Multiple hydrogen bonding sites resolved with FTIR spectroscopy, *Am. Mineral.*, in press.
Peng, Q. and R. E. Cohen, Origin of pyroelectricity in $LiNbO_3$, *Phys. Rev. Lett.* **83**, 220103 (2011).
Peng, S., J. S. Okasinski, J. D. Almer, Y. Ren, L. Wang, W. Yang, and Y. Sun, Real-time probing of the synthesis of colloidal silver nanocubes with time-resolved hihg-energy synchrotron x-ray diffraction, *J. Phys. Chem. C* **116**, 11842-11847 (2012).
Pigott, J. S., D. M. Reaman, and W. R. Panero, Microfabrication of controlled-geometry samples for the laser-heated diamond-anvil cell using focused ion beam technology, *Rev. Sci. Instrum.* **82**, 115106 (2011).
Pravia, M., L. Bai, C. Park, Y. Liu, M. Galley, J. Robinson, and D. Hatchett, Note: Experiments in hard x-ray chemistry: In situ production of molecular hydrogen and x-ray induced combustion, *Rev. Sci. Instrum.* **83**, 036102 (2012).
Pravica, M., L. Bai, and N. Bhattacharya, High-pressure x-ray diffraction studies of potassium chlorate, *J. Appl. Cryst.* **45**, 48-52 (2012).
Pravica, M., L. Bai, C. Park, Y. Liu, M. Galley, J. Robinson, and N. Bhattacharya, Note: A novel method for in situ loading of gases via x-ray induced chemistry, *Rev. Sci. Instrum.* **82**, 106102 (2011).
Pravica, M., M. Galley, C. Park, H. Ruiz, and J. Wojno, A high pressure, high temperature study of 1,1-diamino-2,2-dinitro ethylene, *High Press. Res.* **31**, 80-85 (2011).
Pravica, M., M. Galley, C. Park, H. Ruiz, and J. Wojno, In-situ synchrotron x-ray study of phase transition in melamine under high pressures and high temperatures, *Diamond Rel. Mater.* **20**, 1090-1092 (2011).
Pravica, M., Y. Liu, J. Robinson, Z. Liu, N. Velisavljevic, and M. Galley, A high-pressure far- and mid-infrared study of 1,1-diamino-2,2-dinitroethylene (FOX7), *J. Chem. Phys.*, submitted.
Qin, Z. X., X. J. Chen, C. Zhang, L. Y. Tang, G. H. Zhong, H. Q. Lin, Y. Meng, and H. K. Mao, Vibrational and structural properties of tetramethyltin under pressure, *J. Chem. Phys.*, in press.
Qin, Z. X., C. Zhang, L. Y. Tang, G. H. Zhong, H. Q. Lin, and X. J. Chen, High-pressure phases of a hydrogen-rich compound: tetramethylgermane, *Phys. Rev. B* **86**, 184110 (2012).
Reaman, D. M., Equation of state, diffusivity and deformation in the Fe-Ni alloy system to determine the structure and dynamics of Earth's inner core, *Ph.D. Thesis, Ohio State University* (2011).
Reaman, D. M., H. O. Colijn, F. Yang, and W. R. Panero, Interdiffusion of Earth's core materials to 65 GPa and 2200 K, *Earth Planet. Sci. Lett.* **349-350**, 8-14 (2012).
Reaman, D. M., G. S. Deahn, and W. R. Panero, Predictive mechanism for anisotropy development in the Earth's inner core, *Earth Planet. Sci. Lett.* **321**, 437-442 (2011).
Rose, M. C. and R. E. Cohen, Giant electrocaloric effect around T_c, *Phys. Rev. Lett.* **109**, 18764 (2012).
Ruiz-Fuertes, J., A. Karandikar, R. Boehler, and D. Errandonea, High-pressure melting of tantalum: Optical and scanning electron microscopy evidence of a flat melting curve, *Appl. Phys. Lett.*, submitted.
Sakamaki, T., Y. Wang, C. Park, T. Yu, and G. Shen, Structure of jadeite melt at high pressures up to 4.9 GPa, *J. Appl. Phys.* **111**, 112623 (2012).
Samudrala, G. K., G. Tsoi, and Y. Vohra, Structural phase transitions in yttrium under ultrahigh pressures, *J. Phys.: Cond. Matt.* **24**, 362201 (2012).
Samudrala, G. K. and Y. K. Vohra, Crystallographic phases in heavy rare earth metals under megabar pressures, *J. Phys.: Conf. Series* **337**, 012111 (2012).
Seagle, C. T., E. Cottrell, Y. Fei, D. R. Hummer, and V. B. Prakapenka, Electrical and thermal transport properties of iron and iron-silicon alloy at high pressure, *Proc. Nat. Acad. Sci.*, submitted.
Seagle, C. T., D. Heinz, A. J. Campbell, and V. B. Prakapenka, Melting in the iron-sulfur system at core pressures, *Geophys. Res. Lett.*, submitted.
Sengupta, A., M. Kim, C. S. Yoo, and J. S. Tse, Polymerization of carbon dioxide: A chemistry view of molecular-to-nonmolecular phase transitions, *J. Phys. Chem. C* **116**, 2061-2067 (2012).
Sha, X. and R. E. Cohen, First-principles studies of electrical resistivity of iron under pressure, *J. Phys.: Condens. Matter* **23**, 075401 (2011).
Shen, G., D. Ikuta, S. V. Sinogeikin, Q. Li, Y. Zhang, and C. Chen, Direct observation of a pressure-induced precursor lattice in silicon, *Phys. Rev. Lett.* **109**, 205503 (2012).
Shen, G., Q. Mei, V. B. Prakapenka, P. Lazor, S. V. Sinogeikin, Y. Meng, and C. Park, Effect of helium on structure and compression behavior of SiO_2 glass, *Proc. Nat. Acad. Sci.* **108**, 6004-6007 (2011).
Shu, J., Mineralogy under extreme conditions, *Geosci. Frontiers* **3**, 1-8 (2012).

Shu, J., X. J. Chen, I. M. Chou, W. Yang, J. Hu, R. J. Hemley, and H. K. Mao, Structural stability of methane hydrate at high pressures, *Geosci. Frontiers* **21**, 93-100 (2011).
Singh, A. K., J. Hu, J. Shu, H. K. Mao, and R. J. Hemley, Strength of rhenium from x-ray diffraction experiements under nonhydrostatic compression to 250 GPa, *J. Phys.: Conf. Series* **377**, 012008 (2012).
Singh, A. K. and H. P. Liermann, Strenght and elasticity of niobium under high pressure, *J. Appl. Phys.* **109**, 113539 (2011).
Singh, A. K., H. P. Liermann, and A. Jain, Compression of high-purity silver to 40 GPa in a diamond anvil cell: pressure dependence of strength and grain size from x-ray diffraction data, *Int. J. Plasticity*, submitted.
Singh, A. K., H. P. Liermann, S. K. Saxena, and H. K. Mao, Compressive strength of gold crystallites under pressure up to 60 GPa: observation of crystallite size effect, *J. Appl. Phys.*, submitted.
Skinner, L. B., C. J. Benmore, S. Antao, E. Soignard, S. Amin, E. Bychkov, E. N. Rissi, J. B. Parise, and J. L. Yarger, Structural changes in vitreous $GeSe_4$ under pressure, *J. Phys. Chem. C* **116**, 2212-2217 (2012).
Souza-Neto, N. M., J. Zhao, E. E. Alp, G. Shen, S. Sinogeiken, G. Lapertot, and D. Haskel, Pressure-induced valence instabilities in f-electron systems: Beyond the bond-valence model, *Science*, submitted.
Souza-Neto, N. M., J. Zhao, E. E. Alp, G. Shen, S. V. Sinogeiken, G. Lapertot, and D. Haskel, Reentrant valence transition in EuO at high pressure: Beyond the bond-valence model, *Phys. Rev. Lett.* **109**, 026403 (2012).
Spaulding, D. K., R. S. McWilliams, R. Jeanloz, J. H. Eggert, P. M. Celliers, D. G. Hicks, G. W. Collins, and R. F. Smith, Evidence for a phase transition in silicate melt at extreme pressure and temperature conditions, *Phys. Rev. Lett.* **108**, 065701 (2012).
Stavrou, E., M. Ahart, M. F. Mahmood, and A. F. Goncharov, Correlation between structural and vibrational lengths of Kel F-800 polymeric glass under pressure, *Phys. Rev. B*, submitted.
Stemshorn, A. K. and Y. K. VOhra, Compression of bulk metallic glass $Zr_{57}Cu_{15.4}Ni_{12.6}Al_{10}Nb_5$, *Am. Mineral.* **31**, 287-291 (2011).
Stevens, L. L., D. M. Dattelbaum, M. Ahart, and R. J. Hemley, High-pressure elastic properties of a flourinated copolymer: Poly(chlorotrifluoroethylene-co-vinylidene flouide) (Kel-F 800), *J. Appl. Phys.* **112**, 023523 (2012).
Strobel, T. A., P. Ganesh, M. Somayazulu, P. R. C. Kent, and R. J. Hemley, Novel cooperative interactions and structural ordering in H_2S-H_2, *Phys. Rev. Lett.* **107**, 255503 (2011).
Strobel, T. A., A. F. Goncharov, C. T. Seagle, Z. Liu, M. Somayazulu, V. V. Struzhkin, and R. J. Hemley, High pressure study of silane to 150 GPa, *Phys. Rev. B* **83**, 144102 (2011).
Strobel, T. A., M. Somayazulu, and R. J. Hemley, Phase behavior of H_2+H_2O at high pressures and low temperature, *J. Phys. Chem.* **115**, 4898-4903 (2011).
Subramanian, N., A. F. Goncharov, V. V. Struzhkin, M. Somayazulu, and R. J. Hemley, Bonding changes in hot fluid hydrogen at megabar pressures, *Proc. Nat. Acad. Sci.* **108**, 6014-6019 (2011).
Sun, L., X. J. Chen, J. Guo, P. Gao, Q. Z. Huang, H. Wang, M. Fang, X. Chen, G. Chen, Q. Wu, C. Zhang, D. Gu, X. Dong, L. Y. Wang, K., A. Li, X. Dai, H. K. Mao, and Z. Zhao, Re-emerging superconductivity at 48 K in iron chalcogenides, *Nature* **483**, 67-69 (2012).
Sun, Y., W. Yang, Y. Ren, L. Wang, and C. Lei, Multiple-step phase transformation in silver nanoplates under high pressure, *Small* **7**, 606-611 (2011).
Sun, Z., J. Zhou, H. K. Mao, and R. Ahuja, Peierls distortion mediated reversible phase transition in GeTe under pressure, *Proc. Nat. Aca. Sci.* **16**, 5948-5952 (2012).
Sun, Z., J. S. Zhou, Y. Pan, Z. Zong, H. K. Mao, and R. Ahuja, Pressure-induced reversible amorphization and an amorphous-amorphous transition in $Ge_2Sb_2Te_5$ phase-change memory material, *Proc. Nat. Acad. Sci.* **108**, 10410-10414 (2011).
Tanis, E., A. Simon, O. Tschauner, P. Chow, Y. Xiao, G. Shen, J. M. Hanchar, and M. Frank, Soulubility of xenotime in a 2 M HCl aqueous fluid from 1.2 to 2.6 GPa and 300 to 500 C, *Am. Mineral.* **97**, 1708-1713 (2012).
Tao, R., Y. Fei, and L. Zhang, Experimental determination of siderite stability at high pressure, *Am. Mineral.*, submitted.
Thomas, S. A., G. M. Tsoi, L. E. Wenger, and Y. K. Vohra, Magnetic and structural phase transitions in erbium at low temperatures and high pressures, *Phys. Rev. B* **84**, 144415 (2011).
Thomas, S. M., C. R. Bina, S. D. Jacobsen, and A. F. Goncharov, Radiative heat transfer in a hydrous mantle transition zone, *Earth Planet. Sci. Lett.* **357-358**, 130-136 (2012).
Tschauner, O., B. Kiefer, M. Nicol, S. V. Sinogeikin, R. S. Kumar, and A. L. Cornelius, Lithium hydroxide dihydrate: A new type of icy material at elevated pressure, *J. Chem. Phys.* **134**, 044526 (2011).
Tsoi, G., W. Malone, W. Uhoya, J. E. Mitchell, Y. K. Vohra, L. E. Wegner, A. S. Sefat, and S. T. Weir, Pressure induced superconductiviyt in $Ba_{0.5}Sr_{0.5}Fe_2As_2$, *J. Phys.: Cond. Matt.* **24**, 495702 (2012).

Tulk, C. A., D. D. Klug, A. M. Dos Santos, G. Karotis, M. Guthrie, J. J. Molaison, and N. Pradhan, Cage occupancies in the high pressure structure H methane hydrate: A neutron diffraction study, *J. Chem. Phys.* **136**, 054502 (2012).

Uhoya, W., J. M. Montgomery, G. K. Samudrala, G. Tsoi, Y. Vohra, S. T. Weir, and A. S. Sefat, High-pressure structural phase transitions in chromium-doped $BaFe_2As_2$, *J. Phys.: Conf. Series* **337**, 012016 (2012).

Uhoya, W., G. Tsoi, Y. Vohra, N. Wolanyk, S. M. Rao, M. K. Wu, and S. T. Weir, Simultaneous measurement of pressure evolution of crystal structure and superconductivity in $FeSe_{0.92}$ using designer diamonds, *Europhys. Lett.* **99**, 26002 (2012).

Uhoya, W. O., J. M. Montgomery, G. M. Tsoi, Y. K. Vohra, M. A. McGuire, A. S. Sefat, B. C. Sales, and S. T. Weir, Phase transition and superconductivity of $SrFe_2As_2$ under high pressure, *J. Phys.: Cond. Matt.* **23**, 122201 (2011).

Uhoya, W. O., G. M. Tsoi, Y. K. Vohra, and A. S. Sefat, Structural phase transitions in EuFe2As2 superconductor at low temperatures and high pressures, *J. Phys.: Cond. Matt.* **23**, 365703 (2011).

van Westrenen, W., J. Li, Y. Fei, W. Minarik, J. V. Orman, T. Komabayashi, and K. Funakoshi, In situ determination of magnesiowustite thermal equation of state to 25 GPa and 2073 K, *Phys. Chem. Minerals*, submitted.

Velisavljevic, N., G. N. Chesnut, L. L. Stevens, and D. M. Dattelbaum, Effects of interstitial impurities on the high pressure martensitic □ to □ structural transformation and grain growth in zirconium, *J. Phys.: Cond. Matt.* **23**, 125402 (2011).

Walker, D. D., R., J. Li, and A. Buono, Nonstoichiometry and growth of some Fe carbides, *Phys. Chem. Minerals*, submitted.

Wang, J., W. Yang, S. Wang, X. Xiao, F. De Carlo, Y. Liu, and W. L. Mao, High pressure nano-tomography using an iterative method, *J. Appl. Phys.* **111**, 112626 (2012).

Wang, K., D. Duan, M. Zhou, S. Li, T. Cui, B. Liu, J. Liu, B. Zou, and G. Zou, Structural properties and halogen bonds a cyanuric chloride under high pressure, *J. Phys. Chem. B* **115**, 4639-4644 (2011).

Wang, L., Y. Ding, U. Patel, W. Yang, Z. Xiao, Z. Cai, W. L. Mao, and H. K. Mao, Studying single nanocrystals under high pressure using an x-ray nanoprobe, *Rev. Sci. Instrum.* **82**, 043903 (2011).

Wang, L., B. Liu, H. Li, W. Yang, Y. Ding, S. V. Sinogeikin, Y. Meng, Z. Liu, X. Zeng, and W. L. Mao, Long-range ordered amorphous carbon clusters: A crystalline material with amorphous building blocks, *Science* **337**, 825-828 (2012).

Wang, L., H. Liu, J. Qian, W. Yang, and Y. Zhao, Structural stability and compressibility study for ZnO nanobelts under high pressure, *J. Phys. Chem C* **116**, 2074-2079 (2012).

Wang, L., W. Yang, Y. Xiao, B. Liu, P. Chow, G. Shen, and H. K. Mao, Application of a new composite c-BN gasket assembly for high pressure IXS studies of carbon related materials, *Rev. Sci. Instrum.* **82**, 073902 (2011).

Wang, S., Y. F. Meng, N. Ando, M. Tate, S. Krasnicki, C. S. Yan, Q. Liang, J. Lai, H. K. Mao, S. M. Gruner, and R. J. Hemley, Single-crystal CVD diamonds as small-angle x-ray scattering windows for high pressure research, *J. Appl. Cryst.* **45**, 453-457 (2012).

Wang, S., X. Yu, Z. Lin, R. Zhang, D. He, J. Qin, J. Zhu, J. Han, L. Wang, H. K. Mao, J. Zhang, and Y. Zhao, Synthesis, crystal structure, and elastic properties of novel tungsten nitrides, *Chem. Mater.* **24**, 3023-3028 (2012).

Wang, S., X. Yu, J. Zhang, M. Chen, J. Zhu, L. Wang, D. He, Z. Lin, R. Zhang, K. Leinenweber, and Y. Zhao, Experimental invalidation of phase-transition-induced elastic softening of CrN, *Phys. Rev. B* **86**, 064111 (2012).

Wang, X., F. Tian, L. Wang, X. Jin, D. Duan, X. Huang, B. Liu, and T. Cui, Novel metallic metastable phases of polymeric nitrogen: A first-principles study, *Phys. Rev. Lett.*, submitted.

Wang, Y., J. E. Panzik, B. Kiefer, and K. K. M. Lee, Crystal structure of graphite under room-temperature compression and decompression, *Sci. Reports* **2**, 520 (2012).

Wei, H., C. S. Yoo, J. Y. Chen, and G. Shen, Oxygen-diffusion limited metal combustions in Zr, Ti and Fe foils: Time- and angle-resolved x-ray diffraction studies, *J. Appl. Phys.* **111**, 063528 (2012).

Wenk, H. R., S. Cottaar, C. Tome, B. Romanowicz, and A. McNamara, Deformation in the lowermost mantle: From polycrystal plasticity to seismic anisotropy, *Earth Planet. Sci. Lett.* **306**, 33-45 (2011).

Williams, Q., E. Knittle, H. P. Scott, and Z. X. Liu, The high pressure behavior of micas: Vibrational spectra of muscovite, biotite and phlogopite to 30 Pt, *Am. Mineral.* **97**, 241-252 (2012).

Winterrose, M. L., L. Mauger, I. Halevy, A. F. Yue, M. S. Lucas, J. A. Munoz, H. Tan, Y. Xiao, P. Chow, W. Sturhahn, T. S. Toellner, E. E. Alp, and B. Fultz, Dynamics of Fe atoms across the pressure-induced Invar transition in Pd_3Fe, *Phys. Rev. B* **83**, 134304 (2011).

Xie, M., R. Mohammadi, Z. Mao, M. M. Armentrout, A. Kavner, R. B. Kaner, and S. H. Tolbert, Exploring the high-pressure behavior of superhard tungsten tetraboride, *Phys. Rev. B* **85**, 064118 (2012).

Xu, M., Y. Q. Cheng, L. Wang, H. W. Sheng, Y. Meng, W. G. Yang, X. D. Han, and E. Ma, Pressure tunes electrical resistivity by four orders of magnitude in amorphous $Ge_2Sb_2Te_5$ phase-change memory alloy, *Proc. Nat. Acad. Sci.* **109**, E1055-E1062 (2012).

Yamada, A., Y. Wang, T. Inoue, W. Yang, C. Park, T. Yu, and G. Shen, High-pressure x-ray diffraction studies on the structure of liquid silicate using a Paris-Edinburg type large volume press, *Rev. Sci. Instrum.* **82**, 015103 (2011).

Yamanaka, T., M. Ahart, Y. Nakamoto, Z. G. Ye, H. K. Mao, and R. J. Hemley, Anharmonic atomic vibration in the relaxor ferroelectric $Pb(Mg_{1/3}Nb_{2/3})O_3$ under pressure, *Phys. Rev. B* **86**, 174108 (2012).

Yamanaka, T., W. L. Mao, P. Ganesh, L. Shulenburger, H. K. Mao, and R. J. Hemley, Crystal structures of (Mg, Fe)SiO_3 post-perovskite, *Proc. Nat. Acad. Sci.* **109**, 1035-1040 (2012).

Yamanaka, T., Y. Nakamoto, H. G. Sugita, S. A., H. K. Mao, and R. J. Hemley, Pressure dependence of electron density distribution and dipole moment of $BaTiO_3$ and $KNbO_3$ ferroelectrics, *High Press. Res.*, submitted.

Yamaoka, H., I. Jarrige, N. Tsujii, M. Imai, J. F. Lin, M. Matsunami, R. Eguchi, M. Arita, K. Shimada, H. Namatame, M. Taniguchi, M. Taguchi, Y. Senba, H. Ohashi, N. Hiraoka, H. Ishii, and K. D. Tsuei, Electronic structure of $YbGa_{1.15}Si_{0.85}$ and $YbGa_xGe_{2-x}$ probed by resonant x-ray emission and photoelectron spectroscopies, *Phys. Rev. B* **83**, 104525 (2011).

Yamaoka, H., I. Jarrige, N. Tsujii, A. Kotani, J. F. Lin, S. Tsutsui, F. Honda, R. Settai, Y. Onuki, N. Hiraoka, H. Ishii, and K. D. Tsuei, On the link between valence fluctuations and the suppression of superconductivity in $CeIrSi_3$ under pressure: A resonant x-ray emission spectroscopy study, *J. Phys. Soc. Jpn.* **80**, 124701 (2011).

Yamaoka, H., I. Jarrige, N. Tsujii, J. F. Lin, T. Ikeno, Y. Isikawa, K. Nishimura, R. Higashinaka, H. Sato, N. Hiraoka, H. Ishii, and K. D. Tsuei, Strong coupling between 4f valence instability and 3d ferromagnetism in $Yb_xFe_4Sb_{12}$ studied by resonant x-ray emission spectroscopy, *Phys. Rev. Lett.* **107**, 177203 (2011).

Yang, L., A. Karandikar, and R. Boehler, Flash heating in the diamond cell: Melting curve of rhenium, *Rev. Sci. Instrum.* **83**, 063905 (2012).

Yang, W., X. Huang, R. Harder, I. K. Robinson, and H. K. Mao, Nanoscale strain evolution of a single crystal under high pressure with coherent difraction imaging technique, *Nature Mat.*, submitted.

Yang, W., F. J. Jia, L. Y. Tang, L. J. Li, Z. A. Xu, and X. J. Chen, Structure feature controlling superconductivity in compressed $BaFe_2As_2$, *Phys. Rev. B*, submitted.

Yang, X., Y. Wang, K. Wang, Y. Sui, M. Zhang, B. Li, Y. Ma, B. Liu, G. Zou, and B. Zou, Polymorphism and formation mechanism of nanobipods in manganese sulfide nanocrystals induced by temperature or pressure, *J. Phys. Chem. C* **116**, 3292-3297 (2012).

Ye, Y., D. A. Brown, J. R. Smyth, W. R. Panero, S. D. Jacobsen, Y. Y. Chang, J. P. Townsend, S. M. Thomas, E. H. Hauri, P. Dera, and D. J. Frost, Compressibility and thermal expansion of hydrous ringwoodite with 2.5(3) wt% H_2O, *Am. Mineral.* **97**, 573-582 (2012).

Yoo, C. S., A. Sengupta, and M. Kim, Carbon dioxide carbonates in the Earth's mantle: Implications to the deep carbon cycle, *Angew. Chem. Int. Ed.* **50**, 11219-11222 (2012).

Yoo, C. S., H. Wei, J. Y. Chen, G. Shen, P. Chow, and Y. Xiao, Time- and angle-resolved x-ray diffraction to probe structural and chemical evolution during Al-Ni intermetallic reactions, *Rev. Sci. Instrum.* **82**, 113901-113906 (2011).

Yoo, C. S., H. Wei, R. Dias, G. Shen, J. Smith, J. Y. Chen, and W. Evans, Time-resolved synchrotron x-ray diffraction on pulsed laser heated iron in diamond anvil cells, *J. Phys.: Conf. Series* **377**, 012108 (2012).

Yoshimura, Y., S. T. Stewart, M. Somayazulu, H. K. Mao, and R. J. Hemley, Convergent Raman features in high density amorphous ice, ice VII, and ice VIII under pressure, *J. Chem. Phys. B* **115**, 3756-3760 (2011).

Zaleski-Ejgierd, P., V. Labet, T. A. Strobel, R. Hoffman, and N. W. Ashcroft, WH_n under pressure, *J. Phys.: Cond. Matt.* **24**, 155701 (2012).

Zeng, Q., Y. Ding, W. L. Mao, W. Luo, A. Blomqvist, R. Ahuja, W. Yang, J. Shu, S. V. Sinogeiken, Y. Meng, J. Z. Jiang, and H. K. Mao, Novel alloy of incompatible elements, *Science*, submitted.

Zeng, Q., H. Sheng, Y. Ding, L. Wang, W. Yang, J. Z. Jiang, W. L. Mao, and H. K. Mao, Long-range topological order in metallic glass, *Science* **17**, 1404-1406 (2011).

Zeng, Q., H. W. Sheng, Y. Ding, L. Wang, W. Yang, J. Z. Jiang, W. L. Mao, and H. K. Mao, Metallic glass with long-range orientation order, *Nature*, submitted.

Zeng, Q. S., C. R. Rotundu, W. L. Mao, J. H. Dai, Y. M. Xiao, P. Chow, X. J. Chen, C. L. Qin, H. K. Mao, and J. Z. Jiang, Low temperature transport properties of Ce-Al metallic glasses, *J. Appl. Phys.* **109**, 113716 (2011).

Zeng, Z., L. Wang, X. Ma, S. Qu, J. Chen, Y. Liu, and D. Yang, Improvement in the mechanical performance of Czochralski silicon under indentation by germanium doping, *Scripta Mater.* **64**, 832-835 (2011).

Zha, C. S., Z. Liu, M. Ahart, R. Boehler, and R. J. Hemley, Infrared spectroscopy of hydrogen phase IV, *Phys. Rev. Lett.*, submitted.
Zha, C. S., Z. Liu, and R. J. Hemley, Synchrotron infrared measurements of dense hydrogen to 360 GPa, *Phys. Rev. Lett.* **108**, 146402 (2012).
Zhang, C., X. J. Chen, Y. L. Li, V. V. Struzhkin, H. K. Mao, Q. Zhang, and H. Q. Lin, Predicted superconductivity of solid germane at modest pressure, *Phys. Rev. Lett.*, submitted.
Zhang, D., J. M. Jackson, W. Sturhahn, and Y. Xiao, Local structure variations observed in orthoenstatite at high pressure, *Am. Mineral.* **96**, 1585-1592 (2011).
Zhang, F. X., M. Lang, Z. Liu, and R. C. Ewing, Phase stability of some actinides with brannerite structure at high pressures, *J. Solid State Chem.* **184**, 2834-2839 (2011).
Zhang, F. X., M. Lang, J. M. Zhang, Z. Q. Cheng, Z. X. Liu, J. Lian, and R. C. Ewing, Phase transition and abnormal compressibility of lanthanide silicate with the apatite structure, *Phys. Rev. B* **85**, 214116 (2012).
Zhang, J. L., S. J. Zhang, H. M. Weng, W. Zhang, Y. X. Yang, Q. Q. Liu, S. M. Feng, X. C. Wang, R. C. Yu, L. Z. Cao, L. Wang, W. G. Yang, H. Z. Liu, W. Y. Zhao, S. C. Zhang, X. Dai, Z. Fang, and C. Q. Jin, Pressure-induced superconductivity in topological parent compound Bi_2Te_3, *Proc. Nat. Acad. Sci.* **108**, 24-28 (2011).
Zhang, J. S., J. D. Bass, T. Taniguchi, and A. F. Goncharov, Elasticity of cubic boron nitride under ambient condition, *J. Appl. Phys.* **109**, 063521 (2011).
Zhang, L., Y. Meng, I. Kantor, and W. L. Mao, Experimental evidence for iron inrichment in $(Mg,Fe)SiO_3$ post-perovskite relative to perovskite, *Earth Planet. Sci. Lett.*, submitted.
Zhang, L., Y. Meng, and W. L. Mao, Effect of pressure and composition on lattice parameters and unit-cell voume of $(Fg,Mg)SiO_3$ post perovskite, *Earth Planet Sci. Lett.* **317-138**, 120-125 (2012).
Zhang, R. F., D. Legut, Z. J. Lin, Y. S. Zhao, H. K. Mao, and S. Veprek, Stability and strength of transition-metal tetraborides and triborides, *Phys. Rev. Lett.* **108**, 255502 (2012).
Zhang, R. F., Z. J. Lin, H. K. Mao, and Y. Zhao, Thermodynamic stability and unusual strength of untra-incompressible rhenium nitrides, *Phys. Rev. B* **83**, 060101(R) (2011).
Zhang, S. J., J. L. Zhang, X. H. Yu, J. Zhu, P. P. Kong, S. M. Feng, Q. Q. Liu, L. X. Yang, X. C. Wang, L. Z. Cao, W. G. W. Yang, L., H. K. Mao, Y. S. Zhao, H. Z. Liu, X. Dai, Z. Fang, S. C. Zhang, and C. Q. Jin, The comprehensive phase evolution for Bi_2Te_3 topological compound as function of pressure, *J. Appl. Phys.* **111**, 112630 (2012).
Zhao, J., H. Liu, L. Ehm, Z. Chen, S. V. Sinogeikin, Y. Zhao, and G. Gu, Pressure-induced disordered substitution alloy in Sb_2Te_3, *Inorg. Chem.* **50**, 11291-11293 (2011).
Zhao, Q., G. H. Wen, Z. G. Liu, Y. B. Fan, G. T. Zou, R. K. Zheng, S. P. Ringer, and H. K. Mao, A novel method for the synthesis of dense, crystalline CrO_2 nanowire arrays using AAO template-assisted chemical vapor deposition, *Adv. Mat.*, submitted.
Zhao, X., K. Wang, T. Yan, Y. Yan, B. Zou, J. Yu, and R. Xu, Syntheis and pressure-induced reversible phase transition of a crystalline solid europium germanate $NaEuGeO_4$, *Chin. J. Chem.* **30**, 2066-2072 (2012).
Zhao, X., T. Yan, K. Wang, Y. Yan, B. Zou, J. Yu, and R. Xu, $NaEu_3(GeO_4)_2(OH)_2$: A high-pressure-stable photoluminescent lanthanide germanate, *Eur. J. Inorg. Chem.* **2012**, 2527-2532 (2012).
Zhong, G. H., C. Zhang, G. F. Wu, Z. B. Huang, X. J. Chen, and H. Q. Lin, First-principles investigations on the magnetic property in tripotassium doped picene, *J. Magn. Magn. Mater.*, submitted.
336. Zhu, L., Z. Wang, Y. Wang, Y. Ma, G. Zou, and H. K. Mao, Spiral chain O_4 form of dense oxygen, *Proc. Nat. Acad. Sci.* **109**, 751-753 (2012).
337. Zhu, Q., A. R. Oganov, C. W. Glass, H. K. Mao, S. E. Boulfelfel, P. L. Lee, and W. L. Mao, Structure predictions for molecular crystals using evolutionary algorithms: Methodology and applications, *Proc. Nat. Acad. Sci.*, submitted.
338. Zhuravlev, K. K., A. Goncharov, S. N. Tkachev, P. Dera, and V. Prakapenka, Cubic silicon carbide as a primary pressure calibrant, *Phys. Rev. B*, submitted.
339. Zou, X., B. B. Liu, Q. Li, Z. Li, B. Liu, W. Wu, R. Liu, D. Li, B. Zou, T. Cui, G. Zou, and H. K. Mao, High pressure studies of ß-phase GeO_2 nano particles, *J. Phys. Chem.*, submitted.

B. CDAC Presentations

Abdula, D., K. Nguyen, K. Kang, S. Fong, T. Ozel, D. Cahill, and M. Shim, Influence of defects and doping on optical phonon dynamics in carbon nanotubes, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).
Adams, K., S. D. Jacobsen, Z. Liu, M. Somayazulu, S. M. Thomas, and D. M. Jurdy, Visible and near-infrared reflectivity of solid and liquid methane: application to spectroscopy of Titan's hydrocarbon lakes, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Adams, K. A., S. D. Jacobsen, S. M. Thomas, Z. Liu, M. Somayazulu, and D. M. Jurdy, Visible and infrared reflectivity of solid and liquid methane: Application to hydrocarbon lakes on Titan, *42nd Lunar and Planetary Science Conference* (The Woodlands, TX, March 7-11, 2011).

Ahart, M., Bruillouin scattering study of P-T phase diagram of Ice-VII up to 25 GPa, *2011 GL-GRC Inter-Institution Science Symposium* (Washington, DC, September 19-20, 2011).

Ahart, M., A. F. Goncharov, M. Somayazulu, and R. J. Hemley, Second harmonic generation and high pressure ferroelectricity in $PbTiO_3$(II), *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Al-Khatatbeh, Y., Mechanical strength of zirconia and hafnia phases, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Amulele, G., K. K. M. Lee, and S. Karato, Toward obtaining the experimental constraints on the role of water on melting under the lower mantle conditions, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Amulele, G., K. K. M. Lee, and S. I. Karato, The role of hydrogen in the melting of lower mantle minerals, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Antonangeli, D., T. Komabayashi, G. Morard, G. Fiquet, and Y. Fei, Sound velocity measurements on iron at high pressure and high temperature: An experimental test of the Birch's law, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Antonangeli, D., T. Komabayashi, F. Occelli, G. Fiquet, and Y. Fei, Sound velocity measurements of hcp-Fe at high pressure and high temperature: assessing the limits of the Birch's law, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Armentrout, M., Fiber reinforced composites under pressures: A case study in non-hydrostatic behavior in the diamond anvil cell, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Armentrout, M. A. and A. Kavner, Comparative thermal equations of state for transition metal (Fe, Ni, Co) ringwoodites and implications for the Earth's chemical evolution, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Armentrout, M. M. and A. Kavner, Comparative thermoelastic properties of FeO, NiO, and CoO at high pressures and temperatures: Implications for element partitioning in the mantle, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Baldini, M., V. Struzhkin, A. Goncharov, P. Postorino, and W. Mao, Persistence of Jahn-Teller distortion up to the insulator to metal transition in $LaMnO_3$, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Barkley, M., Classification and topology of hydrogen environments in hydrous minerals: An update, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Berg, C., Laser-driven shock compression of an explosive simulant monolayer, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Berg, C., Picosecnd time-resolved shock complression of energetic materials, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Berg, C. M., Nitro stretch probing of a single molecular layer to monitor shock compression with picosecond time resolution, *17th APS SCCM Conference* (Chicago, IL, July, 2011).

Bernier, J. V., N. R. Barton, D. Farber, H. R. Wenk, M. Kunz, and U. Lienert, Direct observation of phase transitions: In situ diffractin measurements at the crystal scale, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Bi, W., High-Pressure Studies of Structure, Valence, and Magnetism in Europium Metal to 92 GPa, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Bi, W., Magnetism and superconductivity under extreme pressure in rare earth elements (invited), *Advanced Photon Source, Argonne National Laboratory* (Argonne, IL, February 9, 2011).

Bi, W., High-pressure studies of valence and magnetic state in europium metal, *APS March Meeting* (Dallas, TX, Marhc 21-25, 2011).

Bi, W., Pressure-induced structure transitions in europium metal to 92 GPa, *APS March Meeting* (Dallas, TX, Marhc 21-25, 2011).

Bi, W., G. Fabbris, J. Schilling, N. Souza-Neto, D. Haskel, J. Zhao, E. E. Alp, Y. Meng, and A. Alsmadi, High-pressure studies of valance and magnetic state in europium metal, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Bi, W., J. Schilling, Y. Meng, R. Kumar, A. Cornelius, Y. Zhang, C. Chen, and R. Hennig, Pressure-induced structure transition in europium metal to 92 GPa, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Bishop, M., W. Uhoya, G. Tsoi, Y. K. Vohra, A. Sefat, and B. C. Sales, Formation of collapsed tetragonal phase in $EuCo_2As_2$, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Bishop, M., N. Velisavljevic, Z. Liu, and M. Galley, 1,1-diamino-2,2-dinitroethylene under high-pressure-high-temperature, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Boulard, E., W. L. Mao, and C. E. Manning, Imaging carbon-rich melts in the Earth's mantle, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Bower, D., D. R. Hummer, A. Kyono, A. Steele, and J. T. Armstrong, The co-evolution of Fe-,Ti-oxides and other microbially induced mineral precipitates in sandy sediments: understanding the role of microbes in diagenesis *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Brady, N., G. Tsoi, T. Gebre, Y. K. Vohra, and D. Hilton, High-pressure resistivity of $CeCoIn_5$ at low temperatures using four-point probe technique and finite element analysis, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Brown, K., Time-resolved emission spectroscopy of shocked materials, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Brown, K., Emission spectroscopy of shocked materials, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Brown, K. E., Microstates of a shocked polymer, *Shock Compression of Condensed Matter* (June, 2011).

Brown, K. E., Static and shock compression of materials, *Los Alamos National Laboratory* (Los Alamos, NM, December, 2011).

Brown, K. E. and W. Shaw, Optimizing laser-driven flyer plates for studying time-resolved emission of shocked materials, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Cahill, D., Testing the physics of heat conduction in glasses and crystals using high pressure (invited), *Dynamics Phenomena under Extremes Workshops* (Austin, TX, January 26, 2011).

Cahill, D. G., Measuring thermal transport in extreme environments: Thermal conductivity of water ice VII to 20 GPa, *Workshop of Thermal Issues for Hydrogen Energy Systems* (Kyushu University, Fukuoka, Japan, February 3, 2011).

Cahill, D. G., Ultralow termal conductivity and the thermal conductance of interfaces, *Materials Science and Engineering Department Seminar* (Cornell University, Ithaca, NY, March 10, 2011).

Cahill, D. G., Thermal conductance of material interfaces, *Euromat 2011* (Montpellier, France, September 12-15, 2011).

Cahill, D. G., Thermal conductivity and the thermal conductance of interfaces, *MRS Fall Meeting* (Boston, MA, November 28-December 2, 2011).

Chang, Y. Y., Electronic spin transition of iron in dense hydrous magnesium silicate at high pressure, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Chang, Y. Y., Electronic spin transition of iron in dense hydrous magnesium silicate at high pressure, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Chang, Y. Y., S. D. Jacobsen, J. F. Lin, J. Wu, D. J. Frost, S. M. Thomas, P. K. Dera, Y. Xiao, P. Chow, and G. Shen, Electronic spin transition of iron in dense hydrous magnesium silicate phase D at high pressure, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Chen, B., D. Zhang, W. Leng, J. M. Jackson, Y. Wang, T. Yu, J. Liu, and J. Li, Rapid terrestrial core formation from in situ X-ray computed microtomography (invited), *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Chen, X. J., Q. Z. Huang, J. X. Zhu, M. Fang, W. Bao, J. B. Zhang, L. Y. Tang, J. Shu, V. Struzhkin, R. J. Hemley, and H. K. Mao, Ordering driven superconductivity in alkaline iron selenide, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Chidester, B., A high pressure study of the NH_3-H_2 system, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Chopelas, A. and A. Kavner, Raman spectroscopy of orthopyroxene and clinopyroxene at simultaneous highp ressure and temperatures: Implications for the upper mantle, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Clark, A. N., S. D. Jacobsen, S. Sen, Y. Wang, and C. E. Lesher, The effect of hydration on the time-dependent elastic relaxation in vitreous silica: Combined synchrotron microtomography and diamond anvil cell ultrasonic measurements, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Clark, A. N., C. E. Lesher, S. Sen, S. D. Jacobsen, and Y. Wang, The effect of hydration on the anomolous compressibility of vitreous silica characterized by high pressure x-ray microtomography and GHz ultrasonic interferometry, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Cohen, R. E., Band beyond theory for minerals and fluids at high pressure (keynote), *2011 GL-GRC Inter-Institution Science Symposium* (Washington, DC, September 19-20, 2011).

Cohen, R. E., Dynamical Mean Field Theory (DMFT) predictions of an insulator to metal transition in FeO *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Cohen, R. E. and K. Haule, Metallization of FeO at high temperatures and pressures: DFT-DMFT computations and comparisons with experiments, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).
Cohen, R. E., K. Haule, and G. Kotliar, Insulator to metal and magnetic transitions in FeO under high pressure: DFT-DMFT computations, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).
Cottaar, S., M. Li, L. M. Miyagi, A. K. McNamara, B. A. Romanowicz, and H. R. Wenk, Forward modeling the perovskite-postperovskite transition in seismically anisotropic models beneath a slab, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Dalton, A., Investigating extreme states of matter of fast time scales, *2011 GL-GRC Inter-Institution Science Symposium* (Washington, DC, September 19-20, 2011).
Dalton, D. A., Material failure and phase transition at ultrahigh rates (invited), *Dynamics Phenomena under Extremes Workshops* (Austin, TX, January 26, 2011).
Dalton, D. A., Development of fast optical techniques for investigating extreme condensed states, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).
Dalton, D. A., A. F. Goncharov, W. P. Hsieh, and D. Cahill, High P-T thermal conductivity of periclase using an ultrafast pump-probe method, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Dalton, D. A., R. S. McWilliams, M. F. Mahmood, and A. F. Goncharov, Progress towards single shot spectroscopic techniques for time-resolved measurements in the diamond anvil cell, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).
Dalton, D. A., M. Wong, A. F. Goncharov, J. Ojwang, V. V. Struzhkin, Z. Konopkova, and P. Lazor, Thermal emission determination of argon under extreme pressure and temperature, *Dallas, TX, March 21-25*, 2011).
Deng, L., C. T. Seagle, Y. Fei, and A. Shahar, Electrical resistivity of iron at high pressure and high temperature, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Dera, P. K., R. M. Thompson, and R. T. Downs, The compression pathway of quartz, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
DeVreugd, C., M. Ahart, P. Gehring, D. Viehland, and R. J. Hemley, Pressure induced phase transition in FeGa alloys, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).
Dlott, D. D., Shock compression with high time and space resolution (invited), *Dynamics Phenomena under Extremes Workshops* (Austin, TX, January 26, 2011).
Dlott, D. D., Molecular transformations and energy transfer at interfaces (invited), *USC-DOE Conference on Materials for Energy Applications - Experiment, Modeling and Simulations* (Los Angeles, CA, March, 2011).
Dlott, D. D., Heat and electronics at interfaces (invited), *Workshop on Nonlinear Optics and Interfaces* (Erlangen, Germany, April, 2011).
Dlott, D. D., In situ probing by time-resolved vibrational spectroscopy: Shocked materials and energy storage media (invited), *Studium Conference on In Situ Molecular Spectroscopic Technique and Application* (Orleans, France, June, 2011).
Dlott, D. D., Interfaces under extreme conditions (invited), *American Chemical Society National Meeting* (Denver, CO, August, 2011).
Dlott, D. D., Three directional vibrational spectroscopy of molecular energy (invited), *Federation of Analytical Chemistry and Spectroscopy (FACSS) National Meeting* (Reno, NV, 2011).
Dlott, D. D., Interfaces under extreme conditions (invited), *Rice University Department of Chemistry* (Houston, TX, October, 2011).
Dlott, D. D., Experiments probing fundamental mechanisms of energetic material invitation and ignition (invited), *Materials Research Society National Meeting* (Boston, MA, November, 2011).
Dong, J., X. Tang, A. Kavner, and M. Ntam, First-principles calculation of thermal conductivity of silicate perovskite at high pressures and high temperatures, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).
Dong, J., X. Tang, M. C. Ntam, and A. Kavner, First-principles study of lattice thermal conductivity of MgSiO3 perovskite, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Dorfman, S. M. and T. S. Duffy, Iron rich perovskite and post-perovskite: Implications for lower mantle heterogeneities, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Dorfman, S. M., Y. Meng, V. B. Prakapenka, and T. S. Duffy, Compression of Au, Pt, MgO, and NaCl in Ne and He media to 258 GPa, *Consortium for Materials Properties Research in Earth Sciences (COMPRES) Annual Meeting* (Williamsburg, VA, June, 2011).

Driver, K. P., R. E. Cohen, Z. Wu, B. Militzer, P. L. Rios, M. D. Towler, R. J. Needs, and J. W. Wilkins, Quantum Monte Carlo computations of phase stability, equations of state, and elasticity of high-pressure silica, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Duffy, T. S., S. M. Dorfman, V. Prakapenka, and Y. Meng, Internally consistent pressure scale for Au, Pt, Mo, MgO, NaCl and Ne to 2.5 Mbar, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Duffy, T. S. and C. V. Stan, Elastic properties of mantle minerals (invited), *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Dunton, M., Structural transitions in silica and ligand capped silica nanoparticles under pressurse, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Farfan, G., S. Wang, and W. L. Mao, Raman study of opal at high pressure, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Farfan, G. A., S. Wang, E. Boulard, and W. L. Mao, High pressure behavior of 3d transition metal carbonates, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Fei, Y., View planetary differentiation process through high-resolution 3D imaging, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Fei, Y., An integral approach to investigate planetary cores (invited), *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Finkelstein, G., New insights into high-pressure materials from synchrotron-based single-crystal x-ray diffraction, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Finkelstein, G. J., P. K. Dera, and T. S. Duffy, Single-crystal x-ray diffraction of pyrope garnet to 84 GPa, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Finkelstein, G. J., P. K. Dera, C. M. Holl, Y. Meng, and T. S. Duffy, Single-crystal x-raey diffraction of foresterite to 90 GPa, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Finkelstein, G. J., P. K. Dera, Y. Meng, and T. S. Duffy, New insights into the high-pressure behavior of olivine from single-crystal x-ray diffraction (invited), *Single Crystal Diffraction under Extreme Conditions Workshop, Advanced Light Source User's Meeting*, 2011).

Fu, Y., E. Friedman, K. Brown, and D. Dlott, High pressure vibrational spectroscopy of molecular monolayers, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Fultz, B., High temperature thermodynamics and atom vibrations, *TMS Annual Meeting - Brent Fultz Honorary Symposium* (San Diego, CA, February 28, 2011).

Fultz, B., Non-harmonic phonon thermodynamics, *ISIS Seminar, Rutherford-Appleton Laboratory* (United Kingdom, August 16, 2011).

Fultz, B., Non-harmonic phonon thermodynamics and negative thermal expansion, *Spallation Neutron Source Scattering Science Division Seminar* (Oak Ridge National Laboratory, Oak Ridge, TN, December 7, 2011).

Fultz, B., Non-harmonic phonon thermodynamics, *Lawrence Livermore National Laboratory Department Seminar* (Livermore, CA, December 13, 2011).

Gao, P., H. Chen, T. A. Tyson, Z. Liu, J. Bai, L. Wang, J. Y. Choi, and S. W. Cheong, Anomalous phonon behavior in orthorhombic $LuMnO_3$ at low temperature, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-15, 2011).

Gao, P., T. Yu, T. A. Tyson, X. Hong, Z. Chen, S. Ghose, L. Ehm, and Z. Liu, Low temperature structural of $ScMnO_3$, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Gasparov, L., Z. Shirshikova, T. M. Pekarek, J. Blackburn, J. Struzhkin, A. Gavriliuk, R. Rueckamp, and H. Berger, Raman study of the Verwey transition in magnetite at high-pressure and low-temperature: Effect of AI doping, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Gleason, A. E., A. N. Clar, W. L. Mao, and C. E. Lesher, Effect of hydration on elasticity of vitreous silica (invited), *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Gleason, A. E. and W. L. Mao, Static and dynamic elasticity measurements of iron, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Gleason, A. E. and W. L. Mao, Strength of iron to over 200 GPa: Earth's weak inner core, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Gomez Barreiro, J., M. Voltini, J. R. Martinez-Catalan, H. R. Wenk, S. C. Vogel, L. Mancini, and R. Diez-Fernandez, Texture and shape preferred orientation in mylonites developmed under a complex kinematic frame: The Lalin-Forcarei thrust (NW Iberian Massif, Spain), *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Goncharov, A. F., Time domain experiments in the DAC (invited), *Dynamics Phenomena under Extremes Workshops* (Austin, TX, January 26, 2011).

Goncharov, A. F., Time- and space-domain measurements of the thermal conductivity in diamond anvil cells, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Goncharov, A. F., X. J. Chen, S. Lovanov, P. N. Chen, K. D. Litasov, and H. K. Mao, Phase diagram of methane at high pressures and temperatures, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Gooch, M., B. Lv, L. Deng, T. Muramatsu, J. Meen, Y. Xue, B. Lorenz, and C. W. Chu, $Rb_xFe_2Se_2$: A study of superconductivity under high pressure, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Gramsch, S. A., Carnegie-DOE Alliance Center: Education and Outreach (invited), *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Gramsch, S. A., K. U. Hernandez, and M. Somayazulu, Raman spectroscopic studies of water-carbon dioxide mixtures at high pressure, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Gramsch, S. A. and C. T. Prewitt, Structure and crystal chemistry of $FeAlO_3$ at high pressure, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Gu, T., Y. Fei, V. Stagno, S. Qin, and X. Wu, Structure stability of iron phosphides and metal/silicate partition coefficient for phosphorus in early Mars, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Gygi, F., R. Caracas, and R. E. Cohen, Carbon-bearing silicate melts in the deep Earth, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Hamlin, J. J., J. R. Jeffries, N. P. Butch, P. Syers, D. A. Zocco, S. T. Weir, Y. K. Vohra, J. Paglione, and M. B. Maple, Effect of high pressure on transport and structural properties of topological insulator Bi_2Se_3, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Hazen, R. M., R. T. Downs, J. Golden, E. S. Grew, D. Azzolini, and D. A. Sverjensky, Mercury (Hg) mineral evolution: Supercontinent assembly, ocean geochemistry and the terrestrial biosphere, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Hemawan, K., Simulation of microwave plasma discharge in 915 MHz CVD reactor for single crystal diamond deposition, *2011 GL-GRC Inter-Institution Science Symposium* (Washington, DC, September 19-20, 2011).

Hemley, R. J., The Deep Carbon Observatory (invited), *Dynamics Phenomena under Extremes Workshops* (Austin, TX, January 26, 2011).

Hemley, R. J., Developments at CDAC - The Carnegie/DOE Alliance Center: A Center of Excellence in High Pressure Science and Technology (invited), *2011 Stewardship Science Academic Alliances Symposium* (Washington, DC, February 15, 2011).

Hemley, R. J., Effects of extreme environments on materials (invited), *Russian Ministry of Education and Science* (Moscow, Russia, March 1, 2011).

Hemley, R. J., Overview of research at the Geophysical Laboratory (invited), *EFree Scientific Advisory Committee Meeting* (Washington, DC, March 23, 2011).

Hemley, R. J., Chemistry of Planetary Gases, Liquids, and Ices in Extreme Environments, *242nd American Chemical Society National Meeting and Exposition* (Denver, CO, August 28, 2011).

Hemley, R. J., Diamond materials for creating extreme conditions, *Advanced Diamond Science and Technology Meeting* (Detroit, MI, October 31, 2011).

Hemley, R. J., The continuing impacts of dense silica, *International Conference Celebrating the 50th Anniversary of the Synthesis of Stishovite* (Moscow, Russia, November 10, 2011).

Hemley, R. J., Single-crystal diamond: New developments and applications, *23rd International Conference on High Pressure Science and Technology, AIRAPT-23* (Mumbai, India, September 25-30, 2011).

Hemley, R. J., Energy materials in extreme environments (invited), *Bull. Am. Phys. Soc. (APS March Meeting)* (Boston, MA, February 27-March 2, 2012).

Hemley, R. J., Molecules under pressure (invited), *Carlow University* (Pittsburg, PA, April 16, 2012).

Hemley, R. J., Energy materials in extreme environments (invited), *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Hernlund, J. W., K. Ohta, H. Gomi, E. S. Rainey, K. Hirose, S. Labrosse, R. Caracas, A. Kavner, L. Pilon, and C. T. Houser, Preliminary core-mantle boundary heat flux map (invited), *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Hohensee, G., High pressure thermal conductivity measurements of amorphous, crystalline, and alloy materials, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Holl, C., Single-crystal x-ray diffraction of bismuth sillenite (BSO) and its relevance for dynamic compression studies, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Holl, C. M., J. Chadwick, and T. S. Duffy, Mineral collections and modern technology: Roles in geosciences education and research, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Hong, X., Z. Chen, A. Sengupta, A. F. Goncharov, E. L., T. S. Duffy, and D. J. Weidner, COMPRES X-ray beamlines (X17B3 and X17C) for the diamond anvil cell at the National Synchrotron Light Source, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Hou, Y., Y. Lin, and W. L. Mao, X-ray diffraction and Raman spectroscopy study of pressure induced transition in [1,2,3]tetramantane, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Hrubiak, R., High P-T structure and P-V-T equation of state of hafnium, *Consortium for Materials Properties Research in Earth Sciences (COMPRES) Annual Meeting* (Williamsburg, VA, June 2011).
Hrubiak, R., High P-T phases and P-V-T equation of state of hafnium, *SMEC 2011 Meeting* (Belize and Mexico, April-March, 2011).
Hrubiak, R., Thermal conductivity of zirconium at high pressure and temperature in a laser heated DAC, *SMEC 2011 Meeting* (Belize and Mexico, April-March, 2011).
Hrubiak, R., High-pressure x-ray diffraction study of $SrVO_3$ and $CaVO_3$ perovskite oxides, *SMEC 2011 Meeting* (Belize and Mexico, April-March, 2011).
Hrubiak, R., Measuring thermal conductivity of materials under high temperatures and pressures in a laser heated diamond anvil cell, *Advanced School on the New Developments in Field of Snchrotron Radiation* (Brazilian Synchrotron Light Laboratory, Campinas, SP, Brazil, February, 2011).
Hrubiak, R., Thermal conductivity of zirconium at high pressure and temperture in a laser heated DAC, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).
Hrubiak, R., Equations of state of group IVB transition metals (Ti, Zr, Hf) at high temperatures and pressures, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).
Hsieh, W. P., Development of metal film transducers for time-domain thermoreflectance at high pressures, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).
Hsieh, W. P., M. Losego, P. Braun, S. Shenogin, P. Keblinski, and D. Cahill, Testing the minimum thermal conductivity model for amorphous polymers under high pressure, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).
Hsieh, W. P., A. Lyons, E. Pop, P. Keblinski, and D. Cahill, Pressure tuning of the thermal conductance of weak interfaces, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).
Hu, Q., Y. Ding, and H. Sheng, Uncover the nature of cubic-rhombohedral transition in $Fe_{1-x}O$, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).
Huang, H. and Y. Fei, The effect of Si on the melting temperature of iron up to 24 GPa, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Hummer, D., Crystal chemistry of Fe^{3+} in $(Mg,Fe)SiO_3$ perovskite and implications for lower mantle properties, *2011 GL-GRC Inter-Institution Science Symposium* (Washington, DC, September 19-20, 2011).
Hummer, D. R., Y. Fei, and C. T. Seagle, Thermal equation of state of Fe(III) and Al-bearing magnesium silicate perovskite, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Hummer, D. R., A. Kavner, and C. E. Manning, Structure of $CaCO_3$-$CaSiO_3$ melts at high P-T conditions using in situ x-ray diffuse scattering in a Paris-Edinburgh press, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Jackson, M. D., J. G. Moore, H. R. Wenk, and P. J. Monteiro, Al-tobermorite in pyroclastic rock-seawater environments: 1963-1967 Surtsey Tephra and 2000-year-old Roman Baianus Sinus Harbor concrete, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Jacobsen, S. D., Shining light on Earth's deep water cycle at the NSLS (invited), *NSF Site Visit: Consortium for Materials Property Research in Earth Sciences (COMPRES)* (Brookhaven National Laboratory, November 16, 2011).
Jacobsen, S. D. and K. Cockrell, NSF-CAREER outreach at the K-6 level through Project Excite, Center for Talent Development, School of Education and Social Policy at Northwestern University, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Janssen, C., R. Wirth, M. Kienast, L. F. G. Morales, E. Rybacki, H. R. Wenk, and G. H. Dresen, Effects of fluids on faulting within active fault zones - evidence from drill core samples recovered during the San Andreas Fault Observatory at Depth (SAFOD) drilling project, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Jeffries, J., N. P. Butch, S. R. Saha, K. Kirshenbaum, S. T. Weir, Y. K. Vohra, and J. Paglione, Magnetism, superconductivity, and the volume collapse transition in $(Ca_{0.67}Sr_{0.33})Fe_2As_2$ under pressure, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Jeffries, J. R., A. L. Lima Sharma, P. A. Sharma, C. D. Spataru, S. K. McCall, J. D. Sugar, S. T. Weir, and Y. K. Vohra, The behavior of semi-metal Bi_4Te_3 under pressure, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Jenei, Z., M. Lipp, J. H. Klepeis, B. Baer, H. Cynn, W. Evans, C. Park, and D. Popov, High pressure studies of U_3O_8, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Jenei, Z., M. J. Lipp, J. H. P. Klepeis, H. Cynn, W. J. Evans, and C. Park, High pressure/temperature equation of state of gold silver alloys, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Jin, C., J. Zhu, P. P. Kong, S. J. Zhang, J. L. Zhang, S. M. Feng, H. M. Weng, Q. Q. Liu, X. C. Wang, J. L. Zhu, X. H. Yu, L. X. Yang, R. C. Yu, L. Wang, W. G. Yang, S. C. Zhang, X. Dai, and Z. Fang, Superconductivity in Bi_2Te_3 type three dimensional topological compounds induced via pressure, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Jin, C. Q., J. L. Zhang, S. J. Zhang, H. M. Gong, W. Zhang, P. P. Kong, J. Zhu, L. X. Yang, S. M. Feng, Q. Q. Liu, X. C. Wang, R. C. Yu, W. G. Yang, L. Wang, S. C. Zhang, X. Dai, and Z. Fang, Superconductivity in topological parent compound induced via pressure, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Jing, Z., T. Sakamaki, T. Yu, Y. Kono, J. Wang, C. Park, and G. Shen, Density and sound velocity of Fe-S liquids at high pressures, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Kaercher, P., Texture of FeO during phase transition, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Kaercher, P., Crystallographic preferred orientation in FeO through the cubic-to-rhombohedral phase transition, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Kaercher, P., Two-phase deformation of lower mantle mineral analogs, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Kaercher, P. M., B. Militzer, and H. R. Wenk, Ab initio calculations of elastic constants of plagioclase feldspar, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Kaercher, P. M., S. Speziale, L. M. Miyagi, W. Kanitpanyacharoen, and H. R. Wenk, Texture development in FeO across the cubic to rhombohedral phase transition, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Kalita, P., A. Cornelius, K. Lipinska, O. Hemmers, S. Sinogeikin, M. M. Murshed, T. Gesing, and H. Schneider, New structural phase transitions in $PbMBO_4$ complex oxides: Raman spectroscopy and x-ray diffraction studies, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Kanitpanyacharoen, J., In situ laser and resistive heating techniques of Fe and (Mg,Fe)O at high pressure in radial diffraction geometry, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Kanitpanyacharoen, W., In situ laser and resistive heating techniques at high pressure in radial diffraction geometry, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, february 15-17, 2011).

Kanitpanyacharoen, W., Preferred orientation and phase transformation of zirconium under high pressure and temperature, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Kanitpanyacharoen, W., D. Dewhurst, M. Raven, and H. R. Wenk, Texture and anisotropy of shales from the Officer Basin, Western Australia, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Kanitpanyacharoen, W., H. R. Wenk, S. Matthies, and R. Vasin, Self-containing modeling of elastic anisotropy in shale, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Karbasi, A., Thermodynamics of several elements at high pressures, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Karna, S., Y. K. Vohra, G. Samudrala, and G. Tsoi, Electrical characterization of homoepitaxially deposited boron-doped diamond, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Kavner, A., Fiber reinforced coposites under pressure: A case study in non-hydrostaticbehavior in the diamond anvil cell, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Kavner, A. and M. A. Armentrout, High-pressure high-temperature equation of state of B1 cobalt oxide and implications for redox relations in the Earth's lower mantle, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Kavner, A., S. G. John, and D. Walker, Fe isotope fractionation in molten basalt subject to a redox gradient, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Kebukawa, Y., Organic matter in meteorites: Clues to the origin and evolution of the solar system, *2011 GL-GRC Inter-Institution Science Symposium* (Washington, DC, September 19-20, 2011).

Kim, D. Y., R. Scheicher, C. Pickard, R. Needs, and R. Ahuja, Formation of superconducting platinum hydride under pressure: an ab initio approach, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Kono, Y., C. Kenney-Benson, C. Park, G. Shen, and Y. Wang, Viscosity and structure correlations in NaCl and KCl melts at high pressures, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Krasnicki, S., X-ray characterization of large CVD diamond single crystals, *2011 GL-GRC Inter-Institution Science Symposium* (Washington, DC, September 19-20, 2011).

Kumar, R., J. Hamlin, Y. Xiao, S. Sinogeikin, P. Chow, B. Maple, Y. Zhao, and A. Cornelius, Pressure induced superconductivity in LaFeAsO: The role of anionic height and magnetic ordering, 2011).

Lavina, B., P. K. Dera, E. Kim, L. Dobrzhinetskaya, Y. Meng, R. T. Downs, P. F. Weck, S. R. Sutton, Y. Zhao, and E. Alp, Synthesis of a new high-pressure and high-temperature iron oxide, Fe_4O_5, a plausible key player in deep subduction process (invited), *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Lee, K. K. M., Melting at high pressure (invited), *Dynamics Phenomena under Extremes Workshops* (Austin, TX, January 26, 2011).

Lee, K. K. M. and K. Glazyrin, Enstatite chondrites and th density of the lower mantle, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Lee, K. K. M. and A. Wallenta, Into the deep Earth: Using comics as a learning tool, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Li, J., L. Gao, B. Chen, J. Zhao, E. E. Alp, W. Sturhahn, B. Lavina, and P. K. Dera, Carbon content of the core through new windows of the Earth's interior, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Lim, J., Studies of magnetism and superconductivity under extreme pressure, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Lin, J. F., Electronic and elastic properties of iron-containing minerals in Earth's interior, *Dynamic Properties of Earth and Planetary Materials Workshop, Centre Europeen de Calcul Atomique et Moleculaire (CECAM)* (Lausanne, Switzerland, October, 2011).

Lin, J. F., Electronic spin transition of iron in Earth's lower mantle (invited), *The 31st International Conference on the Applications of the mossbauer Effect (ICAME 2011)* (Kobe, Japan, September, 2011).

Lin, J. F., Efficient energy transportation and generation: Iron pnictide superconductors in extreme environments, *Energy Frontier Research in Extreme Environments (EFree) Annual Meeting* (Washington, DC, September, 2011).

Lin, J. F., Elasticity of iron alloysi n Earth's inner core (invited), *The Asia Oceania Geociences Society (AOGS) Meeting* (Taipei, Taiwan, August, 2011).

Lin, J. F., Electronic spin and valence states of iron in the Earth's lower mantle (invited), *The Asia Oceania Geociences Society (AOGS) Meeting* (Taipei, Taiwan, August, 2011).

Lin, J. F., Elasticity of iron alloys in Earth's inner core (invited), *APS User Meeting, Argonne National Laboratory* (Argonne, IL, May 2011).

Lin, J. F., APS upgrade science case: High energy resolution inelastic x-ray scattering (HERIX) (invited), *Argonne National Laboratory* (Argonne, IL, March, 2011).

Lin, J. F., Transition metal iron compounds in extreme environments (invited), *Geophysical Laboratory, Carnegie Institution of Washington* (Washington, DC, January, 2011).

Lin, J. F., Electronic spin transitions of iron in the Earth's deep mantle, *Nassau-Argonne Mossbauer Symposium* (New York, January, 2011).

Lin, J. F., Synchrotron inelastic x-ray scattering at high pressures: Probing electronic, magnetic, elastic, and phonon properties, *Chines Academy of Sciences, Institute of High Energy Physics, Beijing Synchrotron Radiation Facility* (Beijing, China, November 2011).

Lin, J. F., Transition metal iron comounds in extreme environments, *The 6th Asian Conference on High Pressure Research* (Beijing, China, August 12, 2012).

Lin, J. F., Sound velocities of iron alloys in Earth's core, *COMPRES Annual Meeting* (Lake Tahoe, NV, July, 2012).

Lin, J. F., Iron-based compounds in extreme environments, *Superconductors an Strongly Correlated Materials, Energy Frontier Research in Extreme Environments (EFree) Workshop* (Washington, DC, April 21, 2012).

Lin, J. F., Electronic spin transitions of iron in Earth's lower mantle, *Joing Symposium of Misasa-2012 and Geofluid-2* (Okayama University, Misasa, Japan, March 18, 2012).

Lin, J. F., Iron pnictide superconductors in extreme environments: The new iron era, *Energy Frontier Research in Extreme Environments (EFree) Highlight Talk Series* (Washington, DC, January 11, 2012).

Lin, J. F., Z. Mao, C. Lu, S. D. Jacobsen, T. S. Duffy, Y. Y. Chang, D. J. Frost, E. H. Hauri, K. K. Zhuravlev, S. N. Tkachev, and V. Prakapenka, Sound velocities of the transition zone minerals (invited), *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Lin, J. F., S. Speziale, Z. Mao, and H. Marquardt, Electronic spin transitions of iron in the lower-mantle: Potential implications to deep-mantle geophysics and geochemistry, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Lin, Y., L. Zhang, H. K. Mao, P. Chow, Y. Xiao, M. Baldini, J. Shu, and W. Mao, Amorphous diamond - A high-pressure superhard carbon allotrope, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Lipinska, K., O. Hemmers, J. Romann, S. Sinogeikin, P. Kalita, S. Balagopal, and A. Nickens, Synthesis, microstructure and bulk properties of complex nasicon-type ceramics, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Lipp, M., Z. Jenei, J. H. P. Klepeis, B. Baer, H. Cynn, W. Evans, D. Fujino, B. Nolan, J. Wermer, C. Park, and D. Popov, Uranium hydride (UH_3) and deuteride (UD_3) under conditions of high pressure and temperature, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Lipp, M. J., Z. Jenei, D. Ruddle, C. Aracne-Ruddle, H. Cynn, W. J. Evans, Y. Kono, C. Kenny-Benson, and Park., Melting studies of materials in a Paris-Edinburgh cell via radiography, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Liu, J., Tandem magnetic transition in compressed Fe_7C_3, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Liu, J., Elasticity of iron alloys in Earth's inner core, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Liu, J., J. F. Lin, Z. Mao, A. Alatas, L. Gao, J. Zhao, and L. S. Dubrovinsky, Compressional wave velocity of Fe alloys in Earth's core, *COMPRES Annual Meeting* (Williamsburg, VA, June, 2011).

Liu, J. and C. Lu, Sound velocity of iron and iron alloy measured at by high-energy resolution inelastic x-ray scattering (HERIXS), *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Liu, J., B. O. Mysen, Y. Fei, H. K. Mao, R. J. Hemley, and J. Li, Temperature dependent Mossbauer spectra of aluminous perovskite and implications for the Earth's lower mantle, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Liu, Z., Synchrotron FTIR spectroscopy under static and dynamic compression (invited), *Dynamics Phenomena under Extremes Workshops* (Austin, TX, January 26, 2011).

Lu, C., Elasticity of single-crystal pyrpe under high pressure-temperature conditions, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Madhusudhan, N., K. K. M. Lee, and O. Mousis, Comparative characterization of extrasolar super-earths - Interiors, atmospheres, and formation conditions, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Mao, H. K., Studying electronic dynamics under high pressures with synchrotron inelastic x-ray scattering (invited), *Dynamics Phenomena under Extremes Workshops* (Austin, TX, January 26, 2011).

Mao, H. K., Electronic structure and dynamics of elements at high pressures, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Mao, H. K., Advancing the HP-SR capabilities (invited), *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Mao, W. L., Using x-rays to probe high pressure behavior at the nanoscale (invited), *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Mao, W. L., A. E. Gleason, R. Pentcheva, K. Otte, and A. Suzuki, Spin states of FeOOH at high pressure using x-ray emission spectroscopy and DFT calculations, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Mao, W. L., Y. Lin, W. Yang, and J. Wang, Nanoscale x-ray imaging of deep carbon (invited), *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Mao, Z., J. F. Lin, S. Huang, J. Chen, Y. Xiao, and P. Chow, Synchrotron Mossbauer study of Fe-bearing pyrope at high pressures and temperatures, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Mao, Z., J. F. Lin, S. D. Jacobsen, T. S. Duffy, Y. Y. Chang, D. J. Frost, E. H. Hauri, and V. Prakapenka, Elasticity of hydrous ringwoodite in Earth's transition zone, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Marquardt, H., S. Speziale, A. E. Gleason, S. V. Sinogeikin, I. Kantor, and V. Prakapenka, Brillouin scattering x-ray diffraction of argon to 65 GPa and 800 K, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Mauger, L., Anharmonic behavior in Fe near the α-γ structural phase transition, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Mauger, L., Anharmonic behavior in Fe near the α-γ structure phase transition, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Mauger, L., M. Kresch, M. Lucas, J. Munoz, Y. Xiao, and B. Fultz, Anharmonic phonon behavior in □-Fe at temperatures near the structural phase transition, *TMS Annual Meeting - Approaches for Investigating Phase Transformations at the Atomic Scale* (San Dieg, CA, March 2, 2011).

Mauger, Y., Polaron hopping in $LiFePO_4$ at elevated pressures and temperatures, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

McKiernan, K. and S. Amin, High-pressure Brillouin spectroscopy of basaltic glasses and characterizing pressure induced structural changes in glasses and liquids using NMR, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

McWilliams, R. S., New developments in ultra-fast spectroscopy methods for pulsed heating experiments, *Dynamics Phenomena under Extremes Workshops* (Austin, TX, January 26, 2011).

McWilliams, R. S., J. Ciezak-Jenkins, Y. Kadry, V. Prakapenka, M. Mahmood, and A. Goncharov, High-pressure behavior of a novel, nitrogen-rich energetic material, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

McWilliams, R. S., A. F. Goncharov, M. F. Mahmood, and D. A. Dalton, Bridging the gap between static and dynamic compression: An inertial confinement approach to laser heating experiments in the diamond-anvil cell, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Meng, Y., Synchrotron XRD capabilities for research under extreme conditions at HPCAT, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Meng, Y. F., Recent progress in single-crystal CVD diamond growth, *2011 GL-GRC Inter-Institution Science Symposium* (Washington, DC, September 19-20, 2011).

Meng, Y. F., High-temperature/low-pressure annealing of SC-CVD diamond, *2011 GL-GRC Inter-Institution Science Symposium* (Washington, DC, September 19-20, 2011).

Meng, Y. F., Large high-purity fast-grown single crystal cvd diamond, *2011 GL-GRC Inter-Institution Science Symposium* (Washington, DC, September 19-20, 2011).

Meral, C., M. D. Jackson, P. J. Monteiro, and H. R. Wenk, Characterization of mineral assemblages in ancient Roman maritime concrete with synchrotron x-ray techniques, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Miller, R. A., J. M. Jackson, W. Sturhahn, and C. A. Murphy, Phonon density of states and sound velocities of an iron-nickle alloy at high pressure, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Mogk, D. W., R. J. Beane, D. L. Whitney, and K. E. Nicolaysen, Teaching mineralogy, petrology, and geochemistry in the 21st Century: Instructional resources for geoscience faculty, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Montgomery, J., G. Samudrala, and Y. K. Vohra, Homoepitaxial boron doped diamond anvil as heating element in a diamond anvil cell, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Mtam, M. C., J. Dong, X. Tang, and A. F. Goncharov, First-principles calculation of lattice thermal conductivity of $(Mg_xFe_{1-x}O)$ferropericlase at lower mantle conditions, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Munoz, J., Large softening of the phonon partial densities of states of C15 rare-earth-iron compounds, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Munoz, J., Positive vibration entropy of chemical ordering in FeV, *2011 Joint Annual Conference of the National Society of Black Physicists and the National Society of Hispanic Physicists* (Austin, TX, September, 2011).

Munoz, J., Phonon density of states and high pressure thermodynamics of MgB_2, *TMS Annual Meeting - Brent Fultz Honorary Symposium* (San Diego, CA, February 28, 2011).

Munoz, J., Large softening of the phonon partial densities of states of C15 rare-earth-iron compounds, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Murphy, C. A., J. M. Jackson, W. Sturhahn, and C. A. Murphy, Thermoelasticity of hcp-Fe to 171 GPa, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Musfeldt, J. L., Z. Liu, S. Li, J. Kang, C. Lee, P. Jena, J. L. Manson, J. A. Schlueter, G. L. Carr, and M. H. Whangbo, Pressure-induced Jahn-Teller axis switching in $Cu(pyz)F_2(H_2O)_2$, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Musfeldt, J. L., Z. Liu, A. Litvinchuk, T. V. Brinzari, G. L. Carr, J. A. Schlueter, J. L. Manson, and M. H. Whangbo, Pressure-induced local lattice distortions in $Co(dca)_2$, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Ojwang, J. G. O., R. S. McWilliams, and A. F. Goncharov, High pressure-high temperature studies of ammonia, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

Palaich, S. and A. Kavner, Deep sulfate: Insight into the high-pressure behavior of hanksite via Raman spectroscopy and x-ray diffraction, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Panero, W. R., J. R. Smyth, D. M. Reaman, J. S. Pigott, C. T. Unterborn, D. J. Frost, and Z. Liu, The effects of iron and water on elastic properties of ringwoodite from theory and experiment: Constraint on chemical and thermal variations in the transition zone (invited), *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Park, C., Paris-Edinburgh cell applications at 16BM-B white x-ray beamline, *2011 GL-GRC Inter-Institution Science Symposium* (Washington, DC, September 19-20, 2011).

Park, C., C. Kenny-Benson, Y. Kono, G. Shen, T. Yu, T. Sakamaki, Z. Jing, Y. Wang, M. Abd El Qader, J. Baker, R. Kumar, and N. Velisavljevic, New developments in the Paris-Edinburgh cell program at HPCAT, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Parker, S., S. C. Bae, D. Cahill, and S. Granick, The life cycle of individual boiling bubbles: Insights from beyond optical imaging, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Pigott, J., Microfabrication of controlled-geometry samples for the laser-heated diamond-anvil cell using focused ion beam technology, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Pigott, J. S., D. Reaman, and W. R. Panero, Microfabrication of controlled-geometry samples for the laser-heated diamond-anvil cell using focused ion beam technology, *COMPRES Annual Meeting* (Williamsburg, VA, June, 2011).

Pigott, J. S., D. M. Reaman, and W. R. Panero, Microfabrication of controlled-geometry samples for the laser-heated diamond-anvil cell using focused ion beam technology, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Poltorak, D. and W. L. Mao, High pressure study of mixed valence compound $CsAuI_3$, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Potter, R. J., Electronic structure theory-high pressure hydrogenation reactions, *2011 GL-GRC Inter-Institution Science Symposium* (Washington, DC, September 19-20, 2011).

Prakapenka, V., A. F. Goncharov, V. Struzhkin, I. Kantor, M. L. Rivers, and D. A. Dalton, Time-domain x-ray diffraction in the pulsed laser heated diamond anvil cell, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Pray, J. M., Behavior of actinide-bearing materials under extreme conditions, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Queen, D., J. Karel, X. Liu, G. Hohensee, D. Cahill, and F. Hellman, Two level systems in amorphous silicon, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).

Rainey, E. S., A. Kavner, J. W. Hernlund, and L. Pilon, Measuring thermal conductivity at high pressure and temperature in the laser-heated diamond anvil cell, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Rainey, E. S., A. Kavner, J. W. Hernlund, L. Pilon, and M. Veitch, Heat flow in the laser-heated diamond anvil cell and the thermal conductivity of iron-bearing oxides and silicates at lower mantle pressures and temperatures, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Reaman, D., Viscosity constraints of Earth's inner core, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).

Reaman, D., H. O. Colijn, and W. R. Panero, High-pressure, high-temperature diffusion measurements in iron-nickle alloys to 65 GPa, *COMPRES Annual Meeting* (Williamsburg, VA, June, 2011).

Reaman, D. M., G. Daehn, and W. R. Paneron, Inner-core anistotropy: Bridging our understanding between seismology and mineral physics (invited), *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Reaman, D. M., W. R. Panero, and H. Colijn, High-pressure, high-temperature diffusion measurements in iron-nickel alloys to 65 GPa, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Reichmann, H. J., S. D. Jacobsen, and T. Boffa Ballaran, Compositional dependence of elastic moduli for transition-metal oxide spinels, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Sakamaki, T., Y. Kono, Y. Wang, C. Park, T. Yu, Z. Jing, and G. Shen, Sound velocity and structure measurement of silicate glasses under pressure, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Sakamaki, T., T. Yu, Z. Jing, C. Park, G. Shen, and Y. Wang, Density and structure of jadeite melt at high pressure and high temperature, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Saxena, S. K., Application of fast XRD to understanding materials processes (invited), *Dynamics Phenomena under Extremes Workshops* (Austin, TX, January 26, 2011).

Schilling, J. S., How to turn alkali metals into electrides (invited), *HPCAT Workshop* (Argonne National Laboratory, Argonne IL, October 11-12, 2012).

Schilling, J. S., Some recent results in magnetism and superconductivity at high pressure (invited), *Materials Science and Engineering Colloquium* (Cornell University, September 6, 2012).

Schilling, J. S., Interplay between magnetism and superconductivity in elemental rare-Earth metals and related Kondo alloys at high pressure (invited), *Advanced Photon Source Workshop* (Argonne, IL, May 9, 2012).

Seagle, C., Electrical and thermal conductivity of iron and iron-silicon alloy at high pressures, *2011 GL-GRC Inter-Institution Science Symposium* (Washington, DC, September 19-20, 2011).

Seagle, C. T., E. Cottrell, Y. Fei, D. R. Hummer, and V. Prakapenka, Electrical and thermal conductivity of iron and iron-silicon alloy at high pressures (invited), *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Shen, G., HPCAT Program (invited), *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).
Shen, G. and D. Ikuta, Anharmonicity and bonding electrons in silicon under high pressures, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).
Shen, G., S. V. Sinogeikin, P. Chow, Y. Kono, Y. Meng, C. Park, D. Popov, E. Rod, J. Smith, Y. Xiao, and H. K. Mao, Advanced synchrotron techniques at high pressure collaborative access team (HPCAT) (invited), *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Shi, C. Y., Y. Liu, J. Wang, L. Zhang, W. Yang, and W. L. Mao, Formation of iron melt channels in silicate perovskite at Earth's lower mantle conditions, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Shi, Y., W. L. Mao, L. Zhang, W. Yang, J. Wang, Y. Liu, Y. Meng, and J. A. Hayter, High pressure constraints core formation from x-ray nanoscale tomography, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Shibazaki, Y. and Y. Fei, Density comparison between liquid and solid phases in the Fe-FeS system by the sink/float method: Implications for the structural evolution of the cores, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Shirshikova, Z., L. Gasparov, V. Struzhkin, A. Gavriliuk, and H. Berger, Raman study of the verwey transition in magnetite (Fe_3O_4) at high pressure and low temperature: Effect of aluminum doping, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).
Sinogeikin, S. V., E. Rod, C. Kenney-Benson, and G. Shen, Supporting facilities for synchrotron high-pressure/low-temperature research at HPCAT, APS, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Sintubin, M. and H. R. Wenk, Looking at dauphine twins in vein quartz from the high-ardenne slate belt as a potential paleostress indicator, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Smyth, J. R., Y. Ye, and S. D. Jacobsen, Hydration mechanisms, crystal preferred orientation, and anisotropy in the upper mantle and transition zone, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Sorini, A. P., C. C. Chen, S. Wang, W. L. Mao, T. P. Devereaux, and C. C. Kao, Theoretical x-ray spectroscopy for strongly correlated materials at high pressure, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).
Stagno, V., K. L. Crispin, and Y. Fei, Carbon diffusion in solid iron as function of pressure and temperature, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Stan, C. V., V. Prakapenka, and T. S. Duffy, Post-cotunnite phases in the AX2 system: Compression of PbF_2 to 80 GPa, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Stoddard, P. S., K. Pahlevan, S. Tumber, R. Weber, and K. K. M. Lee, Laboratory synthesis of silicate glass spherules: Application to impact ejecta, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Strobel, T., Pressure-induced compound formation in H_2S+H_2, *2011 GL-GRC Inter-Institution Science Symposium* (Washington, DC, September 19-20, 2011).
Sun, L., X. J. Chen, J. Guo, P. Gao, H. Wang, M. Fang, X. Chen, G. Chen, Q. Wu, D. Gu, C. Zhang, X. Dong, X. Dai, H. K. Mao, and Z. Zhao, Pressure-tuned superconductivity of iron chalcogenides, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).
Tang, X., C. W. Li, and B. Fultz, First-principles study of phonon-phonon interaction in FCC metals at high temperatures, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).
Tanis, E. A., A. Simon, O. D. Tschauner, P. Chow, Y. Xiao, J. M. Hanchar, G. Shen, and Y. Zhao, The solubility of Nb-bearing rutile in aqueous fluids containing Albite, NaCl, and NaF from 1-5 GPa and 300-600 C, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Tanis, E. A., A. Simon, O. D. Tschauner, P. Chow, Y. Xiao, and J. M. F. Hanchar, M. R., Partitioning of Nb between rutile and aqueous fluid at high pressures and temperatures, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Tao, R., Y. Fei, and L. Zhang, Petrological and experimental study of the effect of Fe on the stability of dolomite and magenesite in subduction zone, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Terasaki, H., K. Nishida, S. Urakawa, K. Uesugi, Y. Takubo, S. Kuwabara, A. Nakatsuka, M. Hoshino, Y. Kono, Y. Higo, and T. Kondo, Development for sound velocity and density measuremetns of liquid metal at high pressures, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Thomas, S., W. Uhoya, L. Wegner, and Y. K. Vohra, Magnetic phase transition in rare earth metal holmium at low temperatures and high pressures, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).
Thomas, S. M., C. R. Bina, S. D. Jacobsen, and A. F. Goncharov, Tadiative heat transfer in a hydrous transition zone (invited), *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Townsend, J., Mbar-presesure synchrotron-IR of laser-heated materials in the diamond anvil cell, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).
Townsend, J. C., Y. Y., X. Lou, S. Kirklin, J. Doak, A. Issa, S. Tkachev, P. K. Dera, and S. D. Jacobsen, Stability of post-aragonite $BaCO_3$ to 130 GPa and 2000 K, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Uhoya, W., Collapsed tetragonal phae and superconductivity in 112 compounds, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).
Uhoya, W., Anomalous compressibility effects and superconductivity in 1-2-2 iron-base superconductors under high pressure, *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).
Uhoya, W., Simultaneous measurement of pressure evolution of crystal structure and superconductivity in $FeSe_{0.92}$ using designer diamonds, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).
Uhoya, W., N. Wolanyk, G. Tsoi, Y. K. Vohra, S. M. Rao, M. K. Wu, and S. T. Weir, Simultaneous measurement of pressure evolution of crystal structure and superconductivity in $FeSe_{0.8}$ using designer diamonds, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).
Unterborn, C. T., J. A. Johnson, and W. R. Paneron, The distribution of radiogenic elements in stars with and without planetary systems: Implications for dynamics and habitability, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Unterborn, C. T., W. R. Panero, and J. E. Kabbes, Diamond, carbide and carbonate planets, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Uts, I., K. Glazyrin, and K. K. M. Lee, Effect of laser annealing of commn solid pressure media on pressure gradients in a diamond anvil cell, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Wang, J., Single-crystal elastic constants of SiO_2 under pressure -- A comparison between density functional theory and experimental techniques, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).
Wang, J., R. F. Smith, F. Coppari, J. H. Eggert, E. Boehly, G. Collins, and T. S. Duffy, Quasi-isentropic compression of iron and magnesium oxide to 3 Mbar and the Omega Laser Facility, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Wang, L., Ultra-incompressible three dimensional *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).
Wang, S., High pressure chemistry of SiH_4 and H_2O, *American Chemical Society National Meeting* (Denver, CO, August, 2011).
Wang, S., S. Hirai, A. Kemper, M. Baldini, H. Ma, S. Riggs, M. Shapiro, T. Devereaux, I. Fisher, W. Mao, and T. Geballe, High pressure study of mixed valence comound $CsAuI_3$, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2012).
Wang, W., J. Huang, C. Murphy, and D. Cahill, Thermal conductance of interfaces with molecular layers - low temperature transient absorption study on gold nanorods supported on self assembled monolayers, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).
Wang, Y., High pressure: A new dimension in nano dimensional matter, *Oakland University Physics Department* (Rochester, MI, March 10, 2011).
Wang, Y., Graphite under high pressure and room temperature, *Stony Brook University, Department of Geoscience* (Stony Brook, NY, March 3, 2011).
Wang, Y., New superhard carbon polymorph, *Schlumberg* (Houston, TX, January 28, 2011).
Wang, Y., Crystal structure of graphite under room-temperature conpression and decompression, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).
Wang, Y., J. E. Panzik, B. Kiefer, and K. K. M. Lee, Crystal structure of high pressure graphite, *2011 COMPRES Annual Meeting* (Williamsburg, VA, June 14-17, 2011).
Wenk, H. R., Mechanical twinning as stress indicator in fault rocks (invited), *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Wenk, H. R. and J. L. Grimsich, Documenting self organization in quartz: A combined EBSD and laser mass spectrometer investigation of Brazilian agate, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).
Winterrose, M. L., L. Mauger, J. Munoz, and B. Fultz, Pressure induced invar anomaly in Pd_3Fe, *The 6th Annual Nassau-Argonne International Mossbauer Symposium* (Garden City, NJ, January 13, 2011).
Wu, J., Synchrotron mossbauer spectra study of iron-based superconductor of $BaFe_2As_2$ at high pressure and low temperature, *2011 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 15-17, 2011).
Wu, Y., M. Xu, Y. Fei, and Z. Jin, Phase relations in chromite+SiO_2 system at high pressure and high temperature and implication for the origin of coesite bearing chromite, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).
Xia, Y., 16-ID-D high pressure spectroscopy at HPCAT, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Yamanaka, T., S. Kharlamova, A. Kyono, V. Struzhkin, H. K. Mao, and R. J. Hemley, Pressure-induced phase transitions and electron spin state changes in iron-bearing spinels, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Yamanaka, T., A. Kyono, S. Kharlamova, E. Alp, W. Bi, and H. K. Mao, Electron spin transition causing structure transformations of earth's interiors under high pressure, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Yang, F., Y. Lin, and W. L. Mao, Diamondoids under high pressure, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Yang, J., Vibrational and elastic properties of ferromagnesite across the electronic spin pairing tansition of iron, *2012 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 22-23, 2012).

Yang, W., Super-dense phase of BCC-aluminum synthesized by femto second laser shock, *Dynamics Phenomena under Extremes Workshops* (Austin, TX, January 26, 2011).

Yang, W., Development on novel high pressure synchrotron radiation techniques at HPSynC, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Yang, W., HPSynC scientific and technique highlights (invited), *2011 CDAC Annual Review* (Argonne, IL, October 25, 2011).

Yang, W., Strain and composition distribution study under high pressure at nanoscale, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Ye, Y., J. R. Smyth, and S. D. Jacobsen, Crystal structure, thermal expansion of OH-clinohumite & OH-chondrodite: Implications for water in Earth's interior, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Yu, T., Y. Kono, T. Sakamaki, Z. Jing, Y. Wang, and G. Shen, High pressure high temperature elasticity study of sodium disilicate glass, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Yu, T., Y. Kono, T. Sakamaki, Z. Jing, Y. Wang, and G. Shen, Elasticity and structure of sodium disilicated glass at high pressures and high temperatures, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Zepeda-Alarcon, E., J. W. Knight, A. MacDowell, L. M. Miyagi, P. M. Kaercher, W. Kanitpanyacharoen, H. R. Wenk, and Q. C. Williams, Resistive heating in radial geometry diamond anvil cell, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Zhang, C., Carbon speciation and precipitation in C-O-H system under high temperaturea nd pressure, *2011 GL-GRC Inter-Institution Science Symposium* (Washington, DC, September 19-20, 2011).

Zhang, C., Y. Fei, and B. O. Mysen, Carbon speciation and precipitation in C-O-H system at high pressure and temperature, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Zhang, L., Effect of pressure and composition on lattice parameters and unit-cell volume of $(Fe,Mg)SiO_3$ post-perovskite, *2011 GL-GRC Inter-Institution Science Symposium* (Washington, DC, September 19-20, 2011).

Zhang, L., Y. Meng, V. Prakapenka, and W. L. Mao, The phase relations in Earth's mid-lower mantle: constraints from in-situ XRD and quantitative chemical analysis, *Eos Trans. AGU Fall Meet., Suppl.* **92** (2011).

Zhang, L., Y. Meng, W. Yang, L. Wang, W. L. Mao, Q. S. Zheng, W. Liu, R. Xu, and H. K. Mao, In-situ single-crystal structural determination of individual grains of high pressure phases in $(Mg,Fe)SiO_3$ at deep lower mantle, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Zhao, Z., J. F. Lin, S. Huang, J. Chen, Y. Xiao, and P. Chow, Synchrotron Mossbauer study of Fe-bearing pyrope at high pressures and temperatures, *Eos Trans. AGU Fall Meet., Suppl.* **93** (2012).

Zhuravlev, K., A. Goncharov, and V. Prakapenka, New primary pressure calibrants for high pressure and temperature scales: SiC-3C and cBN are possible candidates, *Bull. Am. Phys. Soc. (APS March Meeting)* (Dallas, TX, March 21-25, 2011).

APPENDIX II: CDAC Synchrotron Users/Experiments (APS and NSLS) for 2011-2012

A. HPCAT (APS)

A large part of our annual budget was dedicated to the completion of construction and commissioning of the HPCAT facility. In addition to the 30% membership obtained by CDAC in HPCAT, the support generated by SSAAP funding made possible significant scientific productivity of this state-of-the-art high-pressure facility.

User Name	Affiliations	Project	Dates
H. Rhee H. Cynn S. Sinogeikin	LLNL HPCAT	$CaLi_2$ at low temperature and high pressure	February 2-3, 2011
R. Hrubiak V. Drozd S. Huang	Florida International University	Thermophysical properties and phase diagrams of some elements at extreme conditions	February 4-6, 2011
J. H. Klepeis Z. Jenei	LLNL	EOS of U compounds	February 4-6, 2011
Z. Jing	University of Chicago	*In situ* ultrasonic sound velocity and structural measurements of liquid Fe-S alloys at high pressure and high temperature conditions	February 4-8, 2011
B. Li W. Yang L. Wang H. K. Mao	Jilin University HPSynC Carnegie	High pressure study of Rh-hydrogen system	February 6-8, 2011
J Bradley M. Lipp	LLNL	XES of 4f-metals at high pressure	February 6-12, 2011
W. Yang F. Li L. Wang L. Kong	HPSynC Harbin Institute of Technology	*In situ* high pressure structural transition study of nano-NiO, $Ni(CH_5)_2$, CoF_2, and PYN-PT in DACs	February 4-7, 2011
A. Kyono T. Yamanaka Y. Nakamoto D. Ikuta	Carnegie HPCAT	High-*PT* XRD studies for magnetite, ulvospinel, and chromite	February 9-11, 2011
R. Kumar	University of Nevada – Las Vegas	High *P-T* studies on silver and lead chalcogenides and FeSi alloys	February 9-12, 2011
W. Mao A. Gleason	Stanford University	Elasticity o fFe	February 11, 2011
H. K. Mao B. Li Y. Ding	Carnegie Jilin University HPSynC	High pressure x-ray absorption spectroscopy study of Rh-hydrogen system	February 12-14, 2011
H. Cynn C. Aracne B.Baer S. MacLeod	LLNL Atomic Weapons Establishment, UK	f-metal behavior at high temperatures and high pressures using an external heating	February 12-14, 2011
H. Rhee H. Cynn S. Sinogeikin	LLNL HPCAT	$CaLi_2$ at low temperature and high pressure	February 14-15, 2011
P. Kalita	University of Nevada – Las Vegas	High-pressure XRD of alumino-silicate and related family of ceramics	February 16-17, 2011

T. Yamanaka A. Kyono Y. Nakamoto D. Ikuta	Carnegie HPCAT	Powder diffraction of Fe_2SiO_4, $BiMnO_3$, $YbMnO_3$	February 16-19, 2011
N. Velisavljevic C. Adams	LANL	High pressure melt studies on Ag-Cu alloy	February 16-20, 2011
E. Tanis A. Simon O. Tschauner	University of Nevada – Las Vegas	Quantifying trace elements mass transfer of yttrium and rutile at subduction zone conditions	February 16-22, 2011
R. Chellappa F. Rein	LANL	High pressure reactions in simple organics	February 17-19, 2011
V. Iota-Herbei Y. Zhao X. Yu J. Zhu C. Jin	University of Nevada – Las Vegas LANL Chinese Academy of Scineces	Structural transitions in topological insulators at high pressure	February 19-21, 2011
J. Montgomery S. Thomas G. Samudrala	University of Alabama – Birmingham	High pressure-low temperature phase transformations in iron-based layered superconductors	February 19-22, 2011
W. Yang	HPSynC	Pe cell melting study of semiconductor under pressure	February 20-24, 2011
J. H. Klepeis Z. Jenei	LLNL	EOS of U Compounds	February 23-25, 2011
Z. Dong Y. Song A. Liu	University of Western Ontario	High-pressure study of one-dimensional nanostructured titanium dioxide	February 23-25
H. Mao Y. Ding	Carnegie HPsynC	Electronic phase transition of praseodymium at high pressure	February 24-28, 2011
H. K. Mao B. Li W. Yang Y. Ding L. Wang S. Sinogeikin W. Mao	Carnegie HPSynC HPCAT Stanford University	Advancing the maximum static pressure	February 25-27, 2011
Z. Jenei	LLNL	X-ray radiography of UO_3 in a DAC at room temperature and high pressure	February 26-28, 2011
R. Kumar J. Baker	University of Nevada-Las Vegas	Structural studies of Fe pnictides and related compounds at high pressures	February 26-28, 2011
P. Kalita	University of Nevada – Las Vegas	High-pressure XRD of alumino-silicate and related family of ceramics	February 27-28, 2011
C. S. Yoo M. Kim A. Davidson	Washington State University	Structural studies of simple molecules under high pressure	March 2-4, 2011
Y. Nakamoto S. Kharlamova	Carnegie	High-pressure *in situ* x-ray powder diffraction study of yttrium in the pressure region of superconductivity above 100 GPa	March 2-4, 2011
J. Bradley M. Lipp B. Mattern	LLNL Washington State University	XES of 4f-metlas at high pressure	March 2-11, 2011
N. Velisavljevic D. Preston B. Jensen G. Stevens	LANL NSTec	High pressure XRD of metals	March 4-7, 2011

M. Pravica M. Galley S. Dieguez M. H. Bausch	University of Nevada – Las Vegas	Studies of reactive molecules under extreme conditions	March 4-7, 2011
H. Cynn B. Baer J. H. Klepeis S. Weir	LLNL	Compression behavior of uranium and their compounds at high pressure	March 4-7, 2011
D. Dattelbaum R. Chellappa S. Sinogeikin R. Kumar	LANL HPCAT University of Nevada – Las Vegas	High pressure reactions in simple organics	March 7-10, 2011
J. Jeffries	LLNL	The roles of structure and magnetism in inducing superconductivity in the $(Sr,Ba,Ca)Fe_2As_2$ solid solution	March 7-12, 2011
T. Yu	University of Chicago	Investigation of alkali borate melt structure at high pressure and high temperature	March 10-18, 2011
G. Shen C. S. Yoo J. Y. Chen H. Wei	HPCAT Washington State University	Time resolved XRD on reactive minerals	March 11-14, 2011
O. Tschauner V. Iota-Herbei J. Howard D. Antonio	University of Nevada – Las Vegas	Powder diffraction of lithium nitride (Li_3N)	March 12-13, 2011
Y. Ren L. Wang Z. Nie	ANL HPSynC Northern Illinois University	High pressure XRD studies on the premartensite in Ni_2MnGa single crystals	March 12-14, 2011
J. Wu J. Lin	Chinese Academy of Sciences University of Texas at Austin	High pressure-low temperature XRD studies on hexagonal multiferroic magnanites ($YMnO_3$)	March 12-14, 2011
R. Kumar A. Cornelius	University of Nevada – Las Vegas	Nuclear resonant inelastic x-ray scattering experiments on FeSi, FeAs, and related compounds	March 17-21, 2011
J. Zhou J. Chen W. Yang	University of Texas at Austin HPSynC	Structural response of the post-perovskite $CaPtO_3$ and perovskites $CaIrO_3$ and $CaRuO_3$ under pressure to 80 GPa: Revealing the mechanism for perovskite to post-perovskite transition	March 18-20, 2011
H. K. Mao L. Zhang Y. Shi	Carnegie Stanford University	Fe-Mg partitioning at ultrahigh pressure in perovskite and post-perovskite	March 18-20, 2011
B. Lavina	University of Nevada – Las Vegas	Single crystal diffraction of magnetite and Fe-selenide at high pressure	March 20-22, 2011
G. Shen Y. Meng R. Boehler	HPCAT Carnegie	Melting of Ta at high pressures	March 20-24, 2011
L. Mauger H. Tan J. Munoz H. Smith	Caltech	$LiFePO_4$ at high temperature and pressure	March 21-26, 2011
R. Torchio	ESRF	Structure and magnetism in compressed FeCo alloys	March 23-24, 2011
D. Ikuta	HPCAT	Applications of SXD method to rock thin section	March 24-25, 2011

S. Jacobsen Y. Y. Chang	Northwestern University	Compressibility and stability of phase "D" at high pressures and temperature	March 24-25, 2011
T. Strobel	Carnegie	Tungsten hydride (W in H_2) at high PT, Au in H_2 28 GPa to 40 GPa	March 25-27, 2011
W. Yang X. Huang	HPSynC	Powder diffraction of CoF_3, $BaTiO_3$, $TiSi_2$, PZT, and $Fe(C_5H_5)_2$ under high pressure	March 25-29, 2011
J. F. Lin J. Wu	University of Texas at Austin	Electronic states of iron in mantle minerals: A high-pressure synchrotron Mossbauer study	March 26-29, 2011
M. Pravica L. Bai	Unviersity of Nevada, Las Vegas	High pressure studies of $KClO_3$ and MnO_2	March 28-29, 2011
D. Ikuta	HPCAT	Applications of SXD method to rock thin section	March 30-April 1, 2011
K. Lee Y. Wang Z. Du	Yale University	Silicates at high pressures with XRD and laser heating; graphite at high pressures; melting of MgO	March 30-April 1, 2011
S. Dorfman G. Finkelstein	Princeton University	Valence and spin state of Fe in almandine ($Fe_3Al_2Si_3O_{12}$) composition perovskite and post-perovskite	March 30-April 2, 2011
Y. Lin H. Ma	Stanford University	Single crystal XRD of $MnCO_3$ at high pressure	March 31-April 2, 2011
H. Cynn B. Baer S. MacLeod	LLNL Atomic Weapons Establishment, UK	f-metal behavior at high temperature and high pressure using external heating	April 1-4, 2011
W. Yang L. Kong Z. Yu	HPSynC Harbin Institute of Technology	Powder diffraction of CoF_2, $CoCl_2$, and PZT under high pressure	April 2-4, 2011
H. K. Mao X. J. Chen F. Li A. Gleason	Carnegi HPSynC Stanford University	Detecting magnetic properties of $K_{0.8}Fe_{1.6}Se_2$ and ^{57}Fe-bearing materials by nuclear resonant scattering at high pressures	April 2-8, 2011
H. K. Mao L. Zhang	Carnegie	Fe-Mg partitioning at ultrahigh pressures in perovskite and post-perovskite	April 4-7, 2011
H. Ma	Stanford University	Fe at high pressures using side diffraction	April 4-7, 2011
A. Gleason-Holb	Stanford University	Compression of Fe_2O_3	April 4-7, 2011
X. J. Chen	Carnegie	XRD study of $Sn(CH_3)_4$ at high pressure	April 4-7, 2011
D. Antonio J. Howard C. Booth	University of Nevada – Las Vegas LBNL	XANES of zircon and xenotime K-edges under pressure through the diamonds in a DAC	April 4-8, 2011
C. Holl	Northwestern University	High pressure study of brucite, orthopyroxene, and ruby	April 7-9, 2011
S. Dorfman H. Dong	Princeton University	Continuing study of Au, Pt, MgO, and NaCl to 300 GPa	April 7-9, 2011
R. Kumar	University of Nevada – Las Vegas	Structural studies on Fe pnictides and related compounds at high pressures	April 8-11, 2011
L. Mauger S. Tracy J. Munoz T. Lan	Caltech	$LiFePO_4$ at high temperature and pressure	April 8-11, 2011
J. Piggot D. Reaman C. Unterborn	Ohio State University	Platinum EOS to 100 GPa and 3000 K using controlled geometry samples	April 9-11, 2011
B. Lavina	University of Nevada – Las Vegas	Synthesis and characterization of high *P-T* phases	April 11-12, 2011
O. Shebanova	HPSynC	High-pressure XRD and absorption study of rubidium and molybdenum	April 13-15, 2011

B. Lavina	University of Nevada – Las Vegas	Synthesis and characterization of high *P-T* phases	April 14-15, 2011
X. Yu J. Zhu S. M. Wang B. C. Liu	LLNL Jilin University	X-ray emission study of new Fe base superconductivity under pressure	April 14-17, 2011
P. Dera	University of Chicago	High-pressure single-crystal x-ray microdiffraction investigation of metallocenes	April 15-17, 2011
X. Yu S. Wang	LANL	X-ray microdiffraction study of new Fe base superconductivity under high pressure	April 15-17, 2011
M. Jacobsen	University of Nevada – Las Vegas	High pressure studies of CeCoGe and Ce Pt_2In_7	April 17-20, 2011
A. Gleason	Stanford University	Pressure effect on the magnetic properties of FeOOH	April 17-23, 2011
D. Ikuta	HPCAT	Application of SXD method to multi phase crystals	April 20-22, 2011
M. Armentrout E. Rainey	University of California – Los Angeles	The structural evolution and melting curve of osmium metal	April 20-22, 2011
Y. Vohra G. Tsoy G. Samudrala	University of Alabama – Birmingham	Structural, electrical, and magneitic studies on heavy rare earth metals at high pressures using designer diamond anvils	April 22-24, 2011
J. Howard M. Jacobsen	University of Nevada – Las Vegas	High pressure XRD of Y and YPO_4	April 23-24, 2011
Y. Y. Chang	Northwestern University	Electronic spin transition of iron in dense hydrous magnesium silicate at high pressure	April 23-24, 2011
W. Yang Y. Ding	HPSynC	X-ray emission spectroscopy study of CoF_3 and CoI_2 under high pressure	April 24-26, 2011
H. K. Mao L. Zhang X. J. Chen	Carnegie	Fe-Mg partitioning at ultrahigh pressure in perovskite at post-perovskite	April 24-26, 2011
W. Yang	HPSynC	X-ray powder diffraction under high pressure	April 24-26, 2011
B. Lavina L. Bai	University of Nevada – Las Vegas	Single crystal diffraction at high pressure	June 3-5, 2011
L. Dias M. Kim	Washington State University	Phase transitions of extended carbonyl compound under low temperatures and high pressures	June 3-5, 2011
W. Yang	HPSynC	Large volume pressure study of Se-Te at high pressure and temperature	June 4-7, 2011
W. Yang L. Kong	HPSynC	Powder diffraction of CoI_2, PYNT, and SiO_2 porous samples in DAC	June 5-7, 2011
C. Li J. Zhao Z. Yu	Harbin Institute of Technology	Iron base superconductor and topological insulator under low temperature and high pressure	June 5-7, 2011
Y. Lin S. Hirai	Stanford University	Structural evolution and diamondoids at high pressure and variable temperatures	June 8-10, 2011
M. Ahart C. DeVreugd	Carnegie Virginia Tech	Pressure induced phase transition in FeGa alloys	June 9-11, 2011
R. Chellappa	LANL	High pressure reactions in simple organics	June 11-14, 2011
M. Pravica J. Robinson L. Bai Y. Liu M. H. Bausch	University of Nevada – Las Vegas	Studies of organic molecules and catalysts at high pressure and variable temperature	June 11-15, 2011

J. Carryer D. Antonio B. Stewart	University of Nevada – Las Vegas	High-pressure XRD of CeCoSi	June 15-16, 2011
R. Kumar J. Baker M. Abd El Qader	University of Nevada – Las Vegas	*In situ* thermal conductivity measurement under pressure using Paris-Edinburgh cell	June 15-18, 2011
J. H. Klepeis Z. Jenei	LLNL	EOS of U compounds, f-metal behavior at high pressures	June 15-18, 2011
B. Lavina	University of Nevada – Las Vegas	Single crystal diffraction at high pressure in cryostat	June 16-17, 2011
T. Yu T. Sakamaki Z. Jing Y. Kono	University of Chicago Carnegie	High pressure and high temperature study of sodium disilicate melt structure	June 18-21, 2011
W. Yang L. Wang	HPsynC	Phase transitions of C_{70}, 111 type iron based superconductor, and water under high pressures	June 18-21, 2011
L. Bai M. Galley M. Pravica	University of Nevada – Las Vegas	High pressure XRD studies of oxidizers and reducers	June 20-21, 2011
J. Zhu J. Wu	LANL University of Texas at Austin	The structural phase transition, superconductivity in ferropnictide superconductors at high pressures	June 22-25, 2011
S. Haravifard J. Lang A. Banerjee	ANL University of Chicago	XRD study of $SrCu_2(BO_3)_2$	June 22-25, 2011
C. Park D. Popov	HPCAT	Neutron and x-ray school: High pressure diffraction at 16-BM-D	June 23-25, 2011
D. Ikuta	HPCAT	Single crystal XRD at high pressure	June 23-25, 2011
Z. Jenei	LLNL	X-ray scattering of solid and liquid cerium under high pressure and/or temperature	June 23-27, 2011
H. K. Mao F. Li L. Wang W. Yang S. Sinogeikin Y. Ding	Carnegie HPSynC HPCAT ANL	High-pressure XRD study of glassy carbon and C_{70}	June 25-27, 2011
H. Scott E. Cotter E. Borkholder V. Doczy	Indiana University – South Bend	Powder XRD at high pressure	June 25-27, 2011
T. Yu T. Sakamaki Z. Jing Y. Kono	University of Chicago Carnegie	Ultrasonic elastic wave velocity measurements of silicate melt at high pressure and high temperature	June 29-30, 2011
S. Sinogeikin R. Kumar	HPCAT University of Nevada – Las Vegas	Low temperature structural studies of iron arsenide compounds at high pressures	June 29-July 1, 2011
S. Hirai W. Mao H. Ma W. Yang	Stanford University HPSynC	High pressure powder diffraction of 3-D transition metal oxides	June 29-July 2, 2011
T. Yu T. Sakamaki Z. Jing Y. Wang Y. Kono	University of Chicago Carnegie	*In situ* ultrasonic sound velocity and structural measurements of liquid Fe-S alloys at high pressure and high temperature conditions	June 30-July 3, 2011

L. Kong Z. Yu O. Tschauner	Harbin Institute of Technology University of Nevada – Las Vegas	Powder diffraction of microscale samples with and without diamond cell	July 1-2, 2011
K. Wang	Jilin University	High pressure investigation of zeolite and microporous materials	July 2-4, 2011
H. K. Mao L. Wang W. Yang S. Sinogeikin	Carnegie HPSynC HPCAT	High-pressure XRD study of glassy carbon and C_{70}	July 2-4, 2011
C. Sanloup C. Crepisson	Universite Paris Universite Pierre et Marie Curie, Paris	Structure of molten fayalite up to 7 GPa	July 3-8, 2011
M. Somayazulu	Carnegie	XRD studies of $XeBr_4$, XeI_4, and K_2ReH_9	July 5-8, 2011
W. Yang	HPSynC	High *P-T* study of SeTe melting using Paris-Edinburgh cell	July 8-11, 2011
C. Park	HPCAT	DEV-Combined XANES and XRD study of pressure-induced phase transition in ZnO at room temperature	July 9-10, 2011
H. K. Mao Y. Nakamoto Y. Ding M. Sakata T. Nakase	Carnegie APS Osaka University	High pressure and low temperature *in situ* x-ray powder diffraction study of yttrium	July 9-11, 2011
W. Evans	LLNL	High temperature EOS studies	July 10-12, 2011
Y. Kono C. Park T. Sakamaki	Carnegie HPCAT University of Chicago	Development of high-pressure and high-temperature ultrasonic measurement in Paris-Edinburgh cell apparatus	July 11-16, 2011
W. Yang X. Huang F. Li	HPSynC	EXAFS study of GST system using nano-polycrystalline DACs under high pressure	July 13-15, 2011
B. Lavina L. Bai	University of Nevada – Las Vegas	Synthesis of Fe_4O_5 at high pressure; XRD of Co_3O_4 at high pressures	July 15-16, 2011
Y. Vohra W. Uhoya G. Tsoy	University of Alabama – Birmingham	High pressure-low temperature phase transformations in iron-based layered superconductors	July 15-19, 2011
H. K. Mao L. Zhang	Carnegie	Fe-Mg partitioning at ultrahigh pressure in perovskite and post-perovskite	July 16-19, 2011
Y. Shi W. Mao	Stanford University	En90+Fe,Ni,S at high *P-T* for study of core-mantle interactions	July 16-19, 2011
M. Guthrie G. Karotsis W. Yang	Carnegie HPSynC	XRD of $FePO_4$, MnO_2 at high pressure	July 16-19, 2011
M. Lipp Z. Jenei	LLNL	X-ray scattering of liquid metals (silver-gold alloys) under high temperature and pressure	July 16-22, 2011
B. Zou K. Wang	Jilin University	High pressure studies of selected upramolecular architectures	July 20-22, 2011
P. Dera S. Tkachev	University of Chicago	Single crystal diffraction	July 20-22, 2011
J. Wu	University of Texas at Austin	The crystal structural phase transition in ferropnictide superconductors at high temperatures and low temperature	July 22-25, 2011
H. Cynn S. MacLeod	LLNL Atomic Weapons Establishment, UK	XRD study of Mg at high *P-T*	July 22-25, 2011

T. Sakamaki Z. Jing Y. Wang	University of Chicago	Ultrasonic elastic wave velocity measurements of silicate melt at high pressure and high temperature	July 22-25, 2011
Y. Nakamura	Carnegie	XRD study of yttrium up to megabar pressures	July 27-29, 2011
N. Velisavljevic C. Adams M. Bishop	LANL University of West Georgia	Paris-Edinburgh cell high pressure melt studies on Ag-Cu alloy	July 27-31, 2011
B. Li	HPSynC	Rhodium hydride under high pressure and low temperature	July 27-31, 2011
H. K. Mao L. Zhang	Carnegie	Fe-Mg partitioning at ultrahigh pressure in perovskite and post-perovskite	July 31-August 2, 2011
Y. Shi	Stanford University	En90+Fe,Ni,S at high *P-T* for study of core-mantle interactions	July 31-August 2, 2011
D. Popov	HPCAT	Laue topography	August 1-9, 2011
J. Piggot C. Unterborn	Ohio State University	Thermal EOS of Pt	August 3-9, 2011
M. Armentrout E. Rainey	University of California – Los Angeles	XRD study of Fe and Al oxides at high PT	August 5-7, 2011
N. Velisavljevic D. Dolan G. Stevens	LANL SNL NSTec	High pressure XRD and reflectivity of metals	August 5-9, 2011
Y. Meng G. Shen J. Smith	HPCAT	Development of high pressure melting capabilities	August 7-9, 2011
J. H. Klepeis Z. Jenei	LLNL	EOS of U compounds and transition metal alloys and strength studies of transition metals	August 10-12, 2011
D. Popov	HPCAT	White beam Laue	August 10-13, 2011
D. Ikuta G. Shen	HPCAT	Single crystal XRD at high pressure	August 13-15, 2011
W. Yang	HPSynC	Phase transition of silicon under high pressure	August 13-16, 2011
V. Iota-Herbei D. Antonio A. Cornelius E. Bauer C. Booth	University of Nevada – Las Vegas LANL LBNL	5-f valence fluctuations in superconducting actinide compounds: A XANES study	August 15-19, 2011
H. Sheng A. Cadien Q. Hu S. Flemming	George Mason University	Transformation kinetics of GST at high pressures	August 18-20, 2011
M. Pravica M. Galley J. Robinson Y. Liu L. Bai	University of Nevada – Las Vegas	X-ray induced decomposition of oxidizers	August 19-23, 2011
J. M. Pray J. Liu B. Chen	University of Michigan	Phase transition of pyrochlore	August 20-22, 2011

H. Cynn B. Baer S. Weir S. MacLeod	LLNL Atomic Weapons Establishment, UK	f-metal behavior at high temperature and high pressure using external heating	August 22-25, 2011
W. Yang	HPSynC	High pressure study of silicate	August 23-24, 2011
W. Yang K. Li	HPSynC	High pressure powder diffraction study of $Ge_2Sb_2Te_5$ and $Ln_3Sb_3Zn_2O_{14}$ in DACs	October 7-9, 2011
Z. Jenei J. Y. Chen	LLNL	XRD of transition metal alloys	October 9-11, 2011
L. Marshall J. Cheng	University of Texas at Austin	Experimental verification of the critical V-V bond length for the metallic behavior in normal spinel AV_2O_4 under high pressure	October 12-14, 2011
Z. Jing T. Sakamaki Y. Wang T. Yu C. Park	University of Chicago HPCAT	*In situ* ultrasonic sound velocity and structural measurements of liquid Fe-S alloys at high pressure and high temperature conditions	October 12-16, 2011
W. Yang K. Li F. Li Y. Ding	HPSynC	High pressure powder diffraction study of $Ge_2Sb_2Te_5$ and $Ln_3Sb_3Zn_2O_{14}$ in DACs	October 14-16, 2011
C. Park D. Popov	HPCAT	Developing high-resolution powder XRD at 16-BM-D	October 16-18, 2011
Z. Jing T. Sakamaki Y. Wang T. Yu C. Park	University of Chicago HPCAT	High pressure and high temperature study of sodium disilicate melt structure	October 16-21, 2011
P. Dera L. Bai	University of Chicago University of Nevada – Las Vegas	High resolution powder XRD with diamond cells	October 19-23
M. Lipp	LLNL	X-ray scattering of liquid metals (silver-gold alloys) under high temperature and pressure	October 21-25, 2011
D. Ikuta	HPCAT	Single crystal XRD at high pressure	October 24-25, 2011
W. Yang	HPSynC	High *P-T* study of SeTe melting using Paris-Edinburgh cell	October 26-29, 2011
J. H. Klepeis K. Catalli Z. Jenei	LLNL	EOS of chromium oxides and uranium compounds, and strength studies of transition metal alloys	October 26-29, 2011
W. Yang K. Li F. Li Y. Ding	HPSynC	High pressure powder diffraction study of $Ge_2Sb_2Te_5$ and $Ln_3Sb_3Zn_2O_{14}$ in DACs	October 29-31, 2011
T. Sakamaki Z. Jing Y. Kono C. Park	University of Chicago HPCAT	Ultrasonic elastic wave velocity measurements of silicate melt at high pressure and high temperature	October 29-November 4, 2011
C. Park D. Popov	HPCAT	Bragg-Brentano geometry diffractin set up 16-BM-D	November 2-4, 2011
M. Pravica L. Bai	University of Nevada – Las Vegas	Studies of inorganic oxidizers and reducers under extreme conditions	November 4-6, 2011
D. Ikuta G. Shen	HPCAT	Single crystal XRD at high pressure	November 5-6, 2011

G. Fabris M. Zhernenkov D. Haskel	Washington University at St. Louis ANL	Pressure-induced perovskite to postperovskite transition in ferromagnetic $SrRuO_3$ and concomitant collapse of magnetism	November 6-7, 2011
R. Kumar J. Bake N. R. Bandaru	University of Nevada – Las Vegas	*In situ* thermal conductivity measurements under pressure using Paris-Edinburgh cell	November 6-8, 2011
B. Ling	University of Nevada – Las Vegas	High resolution powder XRD and diamond cels	November 7-8, 2011
B. Lavina T. Kolodziej	University of Nevada – Las Vegas	Synthesis of Fe_4O_5 at high *P-T*, XRD of Co_3O_4 at high pressures	November 9-10, 2011
H. K. Mao Y. Ding J. Wang	Carnegie APS HPSynC	Inelastic scattering of sodium plasmons	November 9-11, 2011
H. Cynn B. Baer S. MacLeod	LLNL Atomic Weapons Establishment, UK	Compression behavior of f-metal and Pt/Au at high temperatures an at high pressures using a DAC	November 9-12, 2011
M. Lipp Z. Jenei H. Cynn	LLNL	X-ray scattering of liquid metal (silver-gold alloys) under high temperature and pressure	November 9-13, 2011
H. K. Mao L. Zhang Y. Meng	Carnegie HPCAT	Fe-Mg partitioning at ultrahigh pressure in perovskite and post-perovskite	November 10-12, 2011
Q. Zheng Y. Lin	Stanford University	AlCe, CeLa,CeMg, ZrCuAgAl metallic glass unde compression; high pressure study of diamondoid	November 10-12, 2011
L. Wang K. Li	HPSynC	High *P-T* study of $Yb_3Sb_3Ni_2O_{14}$	November 10-12, 2011
T. Sharp K. Leinenweber	Arizona State University	Micro XRD of natural silicate perovskite in a shocked chondrite	November 12-14, 2011
W. Evans J. Chen	LLNL	Time-resolved study using dynamic DAC	November 12-14, 2011
F. Li W. Yang V. Struzhkin	HPSynC Carnegie	Low temperature magnetic measuremen of high T_c superconductor in DACs	November 12-15, 2011
Y. Kono	HPCAT	Developments of high pressure generation in Paris-Edinburgh large volume press at 16-BM-B	November 13-14, 2011
N. Velisavljevic C. Adams M. Bishop J. Montgomery	LANL University of West Georgia University of Alabama – Birmingham	Paris-Edinburgh cell high pressure melt studies on Ag-Cu alloy	November 16-19, 2011
J. Jeffries N. Butch	LLNL University of Maryland	Thermal expansion and EOS in URu_2Si_2 at elevated pressure and sub-ambient temperatures	November 16-20, 2011
H. Sheng A. Cadien Q. Hu Y. Meng	George Mason University HPCAT	Melting of Ce at high pressure	November 17-19, 2011
K. More J. Bradley E. Bauer	LLNL	XES of 5f-metal at high pressure	November 18-21, 2011

H. K. Mao L. Zhang Q. Zeng Y. Lin L. Wang K. Li	Carnegie Stanford University HPSynC	Fe-Mg partitioning at ultrahigh pressure in perovskite and postperovskite	November 19-21, 2011
D. Antonio J. Baker	University of Nevada – Las Vegas	*In situ* XRD and high pressure studies on $LaGe_3$, $LaGe_5$, and CuO	November 19-21, 2011
R. Hrubiak S. Saxena	Florida International University	Thermophysical properties and phase diagram of transition metals at high pressure; halfnium, zirconium	November 21-23, 2011
A. Kavner C. Manning	University of California – Los Angeles	Physical and chemical properties of water-rich silica melts	November 21-23, 2011
M. Somayazulu T. Strobel R. J. Potter	Carnegie	XRD of transition metal and main group hydrides under pressure	November 21-23, 2011
Z. Mao	University of Texas at Austin	EOS and phase transition of $MgCO_3$	November 23-26, 2011
W. Yang	HPSynC	High pressure powder diffraction study of metal W Mo, and compounds CeAl, ZrCuAgAl in DACs	November 25-27, 2011
R. Kumar	University of Nevada – Las Vegas	Resonant inelastic x-ray scattering and partial fluorescence yield studies at high pressure and low temperatures on $EuFe_2As_2$	November 25-27, 2011
Y. Kono	HPCAT	Developments of high pressure generation in Paris-Edinburgh large volume press at 16-BM-B	November 25-28, 2011
H. K. Meng L. Zhang Y. Meng	Carnegie HPCAT	Fe-Mg partitioning at ultrahigh pressure in perovskite and postperovskite	November 26-29, 2011
T. Kolodziej	AGH University of Science and Technology	NFS experiments on Fe_4O_5 at high pressure	November 27-29, 2011
S. Haravifard J. Lang A. Banerjee L. Bai	ANL University of Chicago University of Nevada – Las Vegas	XRD study of $SrCu_2(BO_3)_2$	November 27-29, 2011
D. Popov	HPCAT	Topography/tomography	November 28-December 8, 2011
Q. Zhou X. Huang F. Li	Jilin University	*P-V-T* EOS of Pt, Mo	November 29-December 1, 2011
R. Chellappa S. Adak D. Dattelbaum F. Rein	LANL	High pressure reactions in simple organics	December 1-3, 2011
N. Velisavljevic	LANL	High pressure XRD of metals	December 2-4, 2011
J. F. Lin Z. Mao J. Wu	University of Texas at Austin Chinese Academy of Sciences	Spin and valence states of iron in Al-bearing silicate post-perovskite in the Earths lower mantle by synchrotron Mossbauer spectroscopy	December 2-4, 2011
Y. Vohra G. Samudrala G. Tsoy W. Uhoya	University of Alabama – Birmingham	Structural, electrical, and magnetic studies on heavy rare earth metals using designer diamond anvils	December 3-5, 2011

D. Popov	HPCAT	Single crystal development	December 4-5, 2011
S. Wang X. J. Chen	Stanford Carnegie	Synchrotron Mossbauer study of high T_c superconductor TiRbFeSe	December 4-6, 2011
M. Zhernenkov D. Haskel G. Fernandez	ANL Washington University at St. Louis	Pressure-induced perovskite to postperovskite transition in ferromagnetic $SrRuO_3$ and concomitant collapse of magnetism	December 5-6, 2011
R. Kumar	University of Nevada – Las Vegas	Structural studies on Fe pnictides and related compounds at high pressures	December 5-6, 2011
P. Kalita	University of Nevada – Las Vegas	High-pressure XRD of the mullite family of ceramics	December 7-8, 2011
M. Zhernenkov D. Haskel O. Gutfleisch K. Skokov	ANL Leibniz Institute for Solid State and Materials Research, Germany	Interplay between structure and magnetism in giant magneto-caloric $LaFe_{13-x}Si_x$ alloys	December 7-8, 2011
X. Yu S. Wang J. Zhu	LANL	*In situ* high pressure synchrotron x-ray study of vanadium, rhenium, and tungsten nitride	December 8-9, 2011
X. Chen J. Shu P. Dera	Carnegie University of Chicago	High-pressure single crystal XRD study of bismouth ferrite: Exploring multiple phase transitions	December 8-10, 2011
D. Popov	HPCAT	White beam laue	December 8-15, 2011
M. Ahart	Carnegie	Pressure induced phase transition in $PbTiO_3$	December 9-11, 2011
S. Wang H. Ma	Stanford University	High pressure XRD study on mixed-valence compound $CsAuI_3$	December 10-12, 2011
H. Cynn S. MacLeod	LLNL Advanced Weapons Establishment, UK	High-pressure thermal properties of Ti	December 11-13, 2011
L. Bai V. Iota-Herbei	University of Nevada – Las Vegas	Correlated lanthanide intermetallics under pressure	December 12-15, 2011
Bradley. J.	LLNL	RXES of 4f-metals at high pressure	December 12-17, 2011
H. Cynn S. Weir B. Baer M. Lipp S. Sinogeikin S. MacLeod	LLNL HPCAT Advanced Weapons Establishment, UK	Compression behavior of f-metal at high temperatures and at high pressures using a DAC	December 14-17, 2011
W. Yang D. Popov	HPSynC HPCAT	X-ray white laue diffraction on single crystal under high pressure	December 15-19, 2011
L. Bai L. Kong Z. Yu L. Li C. Li H. Liu L. Wang	University of Nevada – Las Vegas Harbin Institute of Technology	Single and powder XRD at high pressure	December 16-18, 2011
M. Guthrie K. Li	Carnegie HPsynC	Over-lithiation of battery cathode lattices by high pressure	December 17-18, 2011

M. Pravica L. Bai	University of Nevada – Las Vegas	Studies of MnO_2 at high pressure using XES	December 17-19, 2011
O. Tschauner	University of Nevada – Las Vegas	Lang topography	December 18-19, 2011
W. Yang K. Li Q. Zeng	HPSynC Stanford University	High pressure powder diffraction study of Sr_2ZrWO_4, (Mg,Fe)SiO_3, CeAl, ArCuAgAl in DACs	December 18-20, 2011
B. Lavina	University of Nevada – Las Vegas	Laue diffraction	February 2-5, 2012
S. Hirai	Stanford University	XRD of manganese oxide	February 3-5, 2012
L. Wang	HPSynC	XAFS test and powder diffraction in DAC	February 3-5, 2012
D. Popov	HPCAT	Development of Laue approach	February 3-7, 2012
M. Lipp	LLNL	4f electron delocalization of lanthanides	February 4-6, 2012
Y. Lin	Stanford University	High-pressure study of tetramantane by XRD	February 4-6, 2012
K. Catalli H. Cynn J. Y. Chen	LLNL	Thermal EOS of high Z metals and metal oxides	February 4-7, 2012
M. Somayazulu	Carnegie	Single crystal diffraction of Xe-H_2 compound	February 6-7, 2012
C. Gu S. H. Shim	Massachusetts Institute of Technology	Spin transition of iron in magnesium silicate glass; high pressure behavior of iron bearing gasses	February 6-9, 2012
M. Guthrie T. Fitzgibbons	Carnegie Pennsylvania State University	Amorphization of unsaturated hydrocarbons	February 8-10, 2012
I. Zibrov S. Stishov F. Elkin	Russian Academy of Sciences	X-ray study of magnetic phase transition in COS_2 at high pressures	February 8-11, 2012
Y. Kono	HPCAT	Development of ultrasonic measurement	February 9-11, 2012
H. Cynn S. Weir B. Baer S. MacLeod	LLNL Atomic Weapons Establishment, UK	5f metals at high pressures and temperatures	
J. Yang	University of Texas at Austin	Spin and valence state of post-perovskite in the Earth's lower mantle	February 9-13, 2012
D. Popov	HPCAT	Single-crystal diffraction	February 11-12, 2012
L. Zhang A. Leary S. Kernion	Carnegie Mellon University	FeCo nanocomposite crystallization at high pressure	February 11-14, 2012
M. Lucas	Air Force Research Laboratory	High pressure crystallization of FeCo based nanocrystalline alloys	February 11-14, 2012
L. Mauger	Caltech	FeCo based amorphous alloys under high pressure and temperature	February 11-15, 2012
J. Cheng	University of Texas at Austin	Monitoring the transition from perovskite to postperovskite structure of $CaIrO_3$ by *in situ* high-pressure synchrotron XRD	February 12-14, 2012
S. Sinogeikin	HPCAT	Development of EOS calibration at high and low temperatures	February 13-14, 2012

L. Shen	University of Illinois – Urbana-Champaign	Structural studies of strongly correlated materials at low temperatures; x-ray emission studies on iron pnictides at high pressures	February 13-17, 2012
Q. Zeng	Stanford University	Power-law scaling of density in metallic glass under high pressure	February 15-17, 2012
J. Baker F. Nasreen S. V. Raju	University of Nevada – Las Vegas	High pressure structural measurement on strongly correlated electron systems	February 15-17, 2012
Y. Kono	HPCAT	Development in x-ray radiography measurement	February 15-17, 2012
A. Cadien	George Mason University	GST metastable phase transitions at high pressure	February 16-17, 2012
L. Shen	University of Illinois – Urbana-Champaign	Mechanical property of metal organic frameworks	February 17-18, 2012
L. Kong C. Li Z. Yu H. Liu	Harbin Institute of Technology	High pressure and low temperature study of $BaTiO_3$	February 17-19, 2012
N. Butch J. Jeffries	LLNL	Spin state of Fe in $(Sr,Ca)Fe_2As_2$ under pressure	February 17-21, 2012
Q. Zheng	Stanford University	Pressure dependence of volume in metallic glass	February 17-21, 2012
W. Yang	HPSynC	High pressure study of powder	February 18-20, 2012
B. Haberl J. Bradby D. Sprouster M. Guthrie	Australian National University Carneige	Silicon XIII	February 19-21, 2012
D. Ikuta	HPCAT	Single crystal XRD at high pressure	Febraury 20-21, 2012
J. Baker	University of Nevada – Las Vegas	High pressure structural studies of vanadium, lanthium, and cerium compound	February 21-24, 2012
M. Somayazulu	Carnegie	Micro-diffraction of alkali-carbon clathrates, xenon-carbon comound and dimethyl aminoboranes	February 22-23, 2012
D. Antonio	University of Nevada – Las Vegas	LaAg XRD	February 22-24, 2012
T. Sakamaki	University of Chicago	Structure measurements of silicate glass at high pressure	February 22-24, 2012
V. Strushkin	Carnegie	Resonant x-ray emission of superconductors at high pressure and low temperature	February 22-26, 2012
J. Wu	University of Texas at Austin	RXES $SrFe_2As_2$	February 22-26, 2012
R. Chellappa N. Mack	LANL	High pressure studies of simple organics	February 23-25, 2012
L. Bai	University of Nevada – Las Vegas	X-ray induced decomposition of organic and inorganic substances	February 24-26, 2012
X. Yu	LANL	Superhard materials	February 24-27, 2012
Q. Zheng H. K. Mao L. Zhang	Stanford University Carnegie	Solid solution alloy formation under high pressure	February 25-27, 2012
J. Wu	University of Texas at Austin	XRD $SrFe_2As_2$	February 29-March 2, 2012
Y. Kono	HPCAT	Developments using PEC	February 29-March 1, 2012

O. Tchauner	University of Nevada – Las Vegas	Lang topography and generic diffraction	February 29-March 3, 2012
V. Iota-Herbei	University of Nevada – Las Vegas	Single crystal diffraction studies of geophysical important materials under pressure, *e.g.* ramestelite	February 29-March 3, 2012
P. Chow	HPCAT	Inelastic scattering post-sample collimator development	February 29-March 4, 2012
Y. Jing Y. Zhang	University of Chicago	Ultrasonic measurements of liquid Fe-S at high pressure	March 1-6, 2012
D. Ikuta	HPCAT	Single crystal XRD at high pressure	March 2-3, 2012
J. Bradley	LLNL	f electron volume collapse	March 2-4, 2012
L. Bai J. Robinson B. Hulsey Y. Liu M. Pravica	University of Nevada – Las Vegas	High pressure studies of $KClO_3$/$NaC1O_3$	March 3-4, 2012
W. Yang X. Lu	HPSynC	Powder diffraction in DAC	March 3-5, 2012
J. Wu	University of Texas at Austin	RXES Ba Fe_2As_2 $SrFe_2As_2$	March 4-6, 2012
Y. Ding	ANL	IXS study of H_2 and Na	March 4-12, 2012
D. Ikuta	HPCAT	Single crystal XRD at high pressure	March 5-6, 2012
J. Jeffries	LLNL	Permanent magnet structure under pressure	March 7-8, 2012
N. Velisavljevic M. Bishop	LANL University of Alabama – Birmingham	Diffraction structural measurements of energetic materials	March 7-9, 2012
H. Cynn C. Aracne	LLNL	EOS of Sm-Co alloys and uranium compounds	March 7-10, 2012
Z. Jenei	LLNL	Cerium in the LVP	March 8-11, 2012
H. K. Mao	Carnegie	IXS study of H_2 and Na	March 8-13, 2012
J. Y. Chen	LLNL	Dynamic DAC study of Bi with XRDs	March 9-11, 2012
W. Evans	LLNL	Time-resolved XRD studies	March 9-11, 2012
D. Ikuta L. Bai	HPCAT University of Nevada – Las Vegas	High pressure and temperature study of single crystal phase transition	March 10-12, 2012
S. Sinogeikin	HPCAT	EOS calibration at low and high temperatures	March 11-12, 2012
L. Wang	HPSynC	X-ray Raman of C_{60}	March 11-13, 2012
C. Sanloup	University of Edinburgh	Structure of molten fayalite at high pressure	March 11-16, 2012
M. Zhernenkov	ANL	Sr_2IrO_4 structure under high pressure	March 12-13, 2012
A. Vailionis A. Rode	Stanford University Australian National University	XRD of olivine	March 13-16, 2012

J. M. Pray J. Liu F. Zhang	University of Michigan	Magnesite formation at depths greater than 150 km in Earth's mantle	March 15-17, 2012
S. Hirai	Stanford University	XRD and XAS of silver oxide	March 16-18, 2012
L. Bai	University of Nevada – Las Vegas	X-ray induced decomposition of organic and inorganic substances	March 16-19, 2012
F. Nasreen	University of Nevada – Las Vegas	RIXS and PFY-XAS of YbO metallics	March 16-19, 2012
E. Boulard S. Wang	Stanford University	Diffraction of graphite at high-pressure	March 17-19, 2012
Q. Zeng	Stanford University	XRD sample evaluation for near future high pressure experiments	March 19, 2012
J. Smith	HPCAT	Single crystal XRD development	March 19-20, 2012
D. Mortensen M. Lipp	University of Washington LLNL	Studying electron delocalization under pressure with x-ray emission f electron correlation rare earths	March 19-24, 2012
Y. Y. Chang J. Townsend	Northwestern University	Synthesis of hydrous post-perovskite	March 21, 2012
T. Strobel O. Kurakevych	Carnegie	Diffraction of Mg-C system under high *P-T* conditions	March 21-23, 2012
O. Tschauner	University of Nevada – Las Vegas	High resolution powder diffraction	March 21-24, 2012
T. Sakamaki	Tohoku University	Structure measurements of liquid bismuth at high pressure	March 21-26, 2012
D. Yu Y. Shu	Yanshan University	Liquid Bi structure under high *P-T*	March 21-26, 2012
L. Zhang	Carnegie	Physical properties of silicates at high *P-T*	March 24-26, 2012
L. Bai	University of Nevada – Las Vegas	Energy-dependent composition studies of oxidizers and reducers	March 24-26, 2012
E. Boulard	Stanford University	XES on rhodochrosite at high pressure	March 24-26, 2012
Y. Ding	APS	XRD of Na at high pressures	March 25, 2012
S. Shieh	HPSynC	XRD study of $ReFe_{0.85}Ir_{0.15}CsO$ series	March 28-29, 2012
K. Li	HPSynC	Study of electronic spin configuration of Co_2^+ in rhombohedral pyrochlore $(La_3Co)Sb_3Co)O_{14}$ under high pressure	March 28-29, 2012
P. Dera	University of Chicago	High pressure single crystal XRD studies of metallocenses	March 28-30, 2012
T. Yu	University of Chicago	Sodium disilicate glass structure measurement	March 28-31, 2012
Z. Liu	University of Chicago	High pressure single-crystal x-ray microdiffraction investigation of s-triazine derivatives	March 29, 2012
L. Kong L. Li	Harbin Institute of Technology	Piezoelectric materials at high pressure	March 29-30, 2012
F. Nasreen	University of Nevada – Las Vegas	PFY-XAS and REXS	March 29-30, 2012
C. Park	HPCAT	Development of high pressure interface cell	March 29-April 3, 2012
G. Finkelstein	Princeton University	Single crystal diffraction of Al_2O_3 at high pressure	March 30-April 1, 2012
M. Lipp	LLNL	Ultrasound f-metal	March 31-April 3, 2012

B. Lavina	University of Nevada – Las Vegas	High pressure study of Fe_4O_5	April 1-3, 2012
Y. Meng	HPCAT	High pressure melting	April 4-6, 2012
Y. Lin F. Yang	Stanford University	High pressure powder diffraction of KFeSe, $CnCh_2CH$, PYNT in DAC	April 4-6, 2012
C. Seagle N. Velisavljevic C. Stevens	SNL LANL NSTec	High pressure XRD and reflectivity of metals	April 4-7, 2012
S. Wang	Stanford University	NFS of iron selenide superconductor at high pressure	April 5-7, 2012
L. Zhang	Carnegie	Physical properties of silicates at high pressure and high temperature	April 5-8, 2012
L. Wang	HPSynC	XRD of ytrium oxide at high pressure	April 6, 2012
Q. Zeng	Stanford University	The composition effect of crystallization in metallic glass	April 6-8, 2012
L. Mauger J. Munoz S. J. Tracy	Caltech	NRIXS in FeTi alloys	April 7-12, 2012
M. Lucas	Air Force Research Laboratory	Anharmonicity of Fe atoms in dilute V-Fe alloys and B_2 FeTi	April 7-14, 2012
M. Armentrout	University of California – Los Angeles	Cobalt and nickel doped olivines	April 8-10, 2012
G. Samudrala N. Brady	University of Alabama – Birmingham	High pressure diffraction studies of Y, VO_2	April 11-15, 2012
T. Strobel	Carnegie	Structure of ne carobn compounds	April 12-14, 2012
O. Kurakevych	Carnegie	Synthesis of Mg-C phases under high pressure and high temperature	April 12-16, 2012
E. Tanis A. Simon	University of Nevada – Las Vegas	XRF of Nb-TiO_2 in aqueous fluid at high pressure and high temperature	April 12-20, 2012
Q. Zheng Z. Zeng	Stanford University Arizona State University	Ultrasonic measurements of metallic glasses under high pressure	April 14-17, 2012
O. Kurakevych M. Somayazulu	Carnegie	Single crystal diffraction of xenon compounds	April 15-20, 2012
G. Stinton M. McMahon S. MacLeod	University of Edinburgh Atomic Weapons Establishment, UK	Thermal properties of Mg at high pressure	April 16-18, 2012
K. Catalli C. Aracne	LLNL	Diffraction of LLNL materials	April 18-21, 2012
H. Cynn	LLNL	5f metal EOS	April 18-21, 2012
V. Struzhkin	Carnegie	*In situ* x-ray emission and XRD with laser heating in FeO under pressure	April 21-22, 2012
L. Zhang	Carnegie	Physical properties of silicates at high pressure and high temperature	April 21-23, 2012
F. Li	HPSynC	High pressure study of $CoCP_2$	April 21-23, 2012
X. Huang S. Jiang	Jilin University	The pressure-induced amorphization of SnBr4 by using high energy XRD	April 23-25, 2012
D. Reaman	University of Chicago	XRD of Ni-SiO_2-Ni	April 23-25, 2012
J. Pigott	Ohio State University	*P-V-T* equations of state using nanofabricated metal/oxide/metal samples	April 23-25, 2012

H. Cynn S. MacLeod	LLNL Atomic Weapons Establishment, UK	Compression behavior of 5f metals under high pressure and high temperature	May 31-June 3, 2012
S. Hirai	Stanford University	High pressure XRD of silver oxide	June 1-3, 2012
L. Kong	HPSynC	Single crystal diffraction	June 1-3, 2012
L. Bai	University of Nevada – Las Vegas	High pressure electronic properties of CrN	June 1-4, 2012
X. J. Chen	Carnegie	Structural properties of $Ba_{1.5}C_{14}H_{10}$ under pressure	June 2-3, 2012
J. Wu	University of Texas at Austin	Ba122	June 3-5, 2012
M. Kim G. Borstad Y. J. Ryu	Washington State University	Electronic phase transitions of extended fluorides under low temperature and high pressure	June 3-7, 2012
L. Zhang	Carnegie	Single-crystal diffraction study of natural minerals	June 7-8, 2012
S. Shieh Z. Mi	HPSynC	High-pressure chromite	June 7-9, 2012
Y. Lin	Stanford University	The effect of pressure on $LiMn_2O_4$	June 7-10, 2012
T. Yu	University of Chicago	Sodium disilicate structure measurement	June 8-12, 2012
Y. Ding J. Wang	ANL HPSynC	High-pressure IXS study of H_2	June 9-17, 2012
P. Kalita	University of Nevada – Las Vegas	High-pressure XRD of ceramics	June 10-11, 2012
X. J. Chen	Carnegie	High pressure powder diffraction study of solid phase transition in DAC	June 10-12, 2012
T. Strobel	Carnegie	Single crystal studies of H_2O-H_2 compound	June 11-14, 2012
P. Syers	University of Maryland	Crystal structure of topological semi-metal Yp+Bi under high pressure in a DAC	June 13-15, 2012
N. Butch	LLNL	YPtBi diffraction under pressure	June 13-16, 2012
M. Lipp	LLNL	Ultrasound of cerium under pressure and temperature	June 13-17, 2012
P. Kalita	University of Nevada – Las Vegas	High pressure XRD of ceramics	June 14-15, 2012
L. Kong	HPSynC	High pressure study of piezoelectric materials near MPB	June 15-16, 2012
A. Plonka	University of Chicago	High pressure gas absorption in MOF	June 15-17, 2012
Z. Zhao W. Mao	Stanford University	High pressure XRD measurements on AgTe	June 15-17, 2012
Y. Kono	HPCAT	Developments of PEC	June 17-19, 2012
K. Li	HPsynC	High pressure powder diffraction study of solid phase transition in DAC	June 17-19, 2012
W. Kanitpanyacharoen E. Zapeda-Alarcon	University of California – Berkeley	Preferred orientation and phase transformation of olivine and enstatite	June 17-19, 2012
J. Wu	University of Texas at Austin	Ba122	June 20-22, 2012
S. Smith A. Stemshorn	University of Alabama – Birmingham	Devitrification of metallic glass under high pressure	June 20-23, 2012
J. Jeffries	LLNL	*P-T* phase boundary of the volume collapse in $(Ca,Sr)Fe_2As_2$ under pressure	June 20-23, 2012

Y. Lin T. Fitzgibbons	Stanford University Pennsylvania State University	Ultrahard carbon phase made from SWCNT	June 20-23, 2012
H. Cynn S. MacLeod	LLNL Atomic Weapons Establishment	Compression study of 5f and 4f metals and their compounds	June 22-25, 2012
Y. Kono	HPCAT	Developments in Paris-Edinburgh cell	June 23-July 1, 2012
D. Ikuta T. Yamanaka	HPCAT Carnegie	Structure change of $SrTiO_3$ and $PbTiO_3$ under high pressure by single crystal diffraction study	June 27-29, 2012
H. Cynn J. H. Klepeis	LLNL	Compression study of 5f metal and compounds under extreme conditions	June 27-30, 2012
Z. Jenei J. H. Klepeis	LLNL	EOS of uranium compounds under extreme conditions	June 29-July 2, 2012
O. Tschauner	University of Nevada – Las Vegas	Powder diffraction	June 29-July 2, 2012
J. Bourguille	Laboratoire des Sciences des Procedes et des Materiaux, France	Powder materials Zrn	June 30-July 2, 2012
Y. Liu	University of Nevada – Las Vegas	Studies of x-ray indiced chemical reactions in various compound	June 30-July 4, 2012
D. Haskel G. Fabbris	ANL Washington University at St. Louis	XES Tb	June 30-July 4, 2012
J. Mardegan	University of Campinas	High pressure study of 4l local moment in Tb metal across the volume collapse transition	June 30-July 4, 2012
L. Bai J. Robinson	University of Nevada – Las Vegas	X-ray study decomposition of nitrogen containing compounds	July 1-4, 2012
W. Yang	HPSynC	Powder diffraction under high pressure	July 2-3, 2012
Q. Zeng Z. Zeng	Stanford University	The effect of composition on pressure-induced devitrification in metallic glasses	July 2-4, 2012
D. Ikuta	HPCAT	Single crystal diffraction study	July 3-4, 2012
W. Yang	HPSynC	High pressure diffraction of solid phase transition	July 5-6, 2012
L. Bai M. H. Bausch J. Robinson	University of Nevada – Las Vegas	X-ray induced decomposition of nitrogen contained compounds	July 5-6, 2012
A. Kavner C. Manning D. Hummer	University of California – Los Angeles	High *P-T* behavior of silica carbonate liquid phase	July 5-8, 2012
D. Ikuta	HPCAT	Single crystal diffraction study	July 6-7, 2012
F. Nasreen D. Antonio	University of Nevada – Las Vegas	High pressure XRD in Yb organometallic systems	July 6-8, 2012
L. Wang Y. Lin M. Feng	HPSynC Stanford University Jilin University	Total x-ray scattering of fullerenes at high pressure	July 8-12, 2012
D. Mortensen	University of Washington	4f electron delocalization	July 11-12, 2012
T. Strobel V. Rozsa	Carnegie Hillsdale College	EOS for organic clathrate	July 12-13, 2012
B. Li	HPSynC	High pressure study of Cr	July 14-15, 2012
L. Zhang	Carnegie	Physical properties of silicates at high pressure	July 14-16, 2012

T. Strobel	Carnegie	Single crystal XRD of H_2-H_2O clathrate	July 14-17, 2012
A. Leary V. DeGeorge M. Lucas I. Halevy	Carnegie Mellon University Air Force Research Laboratory NRCN ISrael	Nanocrystallization of magnetic materials under pressure	July 14-17, 2012
M. Diaz Michelena	INTA	Titanomagnetites diffraction in temperature and pressure	July 14-18, 2012
M. Somayazulu	Carnegie	Xenon chemistry	July 15-17, 2012
J. F. Lin	University of Texas at Austin	X-ray emission spectroscopy of iron	July 15-19, 2012
W. Yang	HPSynC	Laser heating and XRD	July 16-19, 2012
K. Li	HPSynC	High pressure study of the structure stability of pyrochlore-type complex oxides	July 18-20, 2012
L. Zhang	Carnegie	Physical properties of mantle silicates at high pressure	July 19-21, 2012
Q. Zeng Z. Zeng	Stanford University	Composition effect on pressure-induced crystallization in metallic glass	July 19-21, 2012
S. Wang	Stanford University	Structure study of cold-compressed graphite	July 19-21, 2012
D. Ikuta	HPCAT	Single-crystal XRD at high pressure	July 20-22, 2012
K. Kothapalli	University of Nevada – Las Vegas	Fe_4O_5 diffraction	July 20-23, 2012
Q. Zeng	Stanford University	Volume of metallic glass under high pressure	July 20-23, 2012
Z. Zeng	Stanford University	Bulk modulus of BMGs under high pressure	July 20-27, 2012
B. Lavina	University of Nevada – Las Vegas	Fe_4O_5 high pressure stability	July 21-23, 2012
J. Wu	University of Texas at Austin	$SrFe_2As_2$ SMS	July 21-24, 2012
Z. Zhao	Stanford University	High pressure XRD study of VO_2	July 22-24, 2012
Q. Zeng	Stanford University	Volume of metallic glass under high pressure	July 23-24, 2012
J. Smith	HPCAT	EOS of epsilon iron	July 23-25, 2012
R. Liu Q. Li	Jilin University	High pressure phase transition of VO_2	July 23-25, 2012
Q. Zeng Z. Zeng	Stanford University	Volume of metallic glass under high pressure	July 23-27, 2012
F. Nasreen D. Antonio D. Van Gennep	University of Nevada – Las Vegas HiPSEC	High pressure XANES measurement on U_2Zn_{17}	July 25-26, 2012
S. Jacobsen	Northwestern University	Comparative compressibility of BCN materials	July 26-27, 2012
Y. Y. Chang X. Liu	Northwestern University	High-pressure compression of four type diamonds	July 26-28, 2012
H. Cynn D. Ikuta	LLNL HPCAT	Single crystal diffraction of spinel and olivine at high pressure	July 26-29, 2012
S. V. Raju L. Bai	University of Nevada – Las Vegas	Low temperature of nuclear for scattering of Fe27 enriched FeSi, FeSe alloys under high pressure	July 26-29, 2012

D. Sneed J. Robinson	HiPSEC University of Nevada – Las Vegas	X-ray decomposition studies of nitrogen containing materials	July 27-30, 2012
S. Gramsch N. Valdez	Carnegie Colorado College	High pressure study of Fe_2SiO_5	July 28, 2012
V. Drozd K. Lazars	Florida International University	Thermodynamics of elements at high pressure and temperature	July 28-30, 2012
L. Bai	University of Nevada – Las Vegas	High pressure study of tyrrellite	July 29-31, 2012
A. Gavriliuk	Russian Academy of Sciences	Spin crossover at high pressure in transition metal oxides	July 29-August 2, 2012
Y. Kono	HPCAT	Developments of viscosity measurement in PEC	July 30-31, 2012
J. Robinson D. Sneed Q. Smith L. Bai	University of Nevada – Las Vegas	X-ray decomposition of $KClO_3$	August 1-3, 2012
S. V. Raju	HiPSEC	Thermal conductivity and electrical resistivity measurement under pressure	August 1-4, 2012
Y. Y. Chang X. Liu	Northwestern University	Comparative compressibilities of c-BCN single crystal	August 3-5, 2012
V. Mktchyan	University of Nevada – Las Vegas	High-pressure Paris-Edinburgh cell technique development	August 1-7, 2012
J. Baker	HiPSEC	Thermal conductivity and electrical resistivity measurements under pressure	August 1-7, 2012
N. Velisavljevic	LANL	High pressure electrical and thermal studies of Paris-Edinburgh cell	August 1-7, 2012
E. Tanis	University of Nevada – Las Vegas	SXRF of Nb-TiO_2 at high pressure and high temperature	August 2-6, 2012
A. Simon	HiPSEC	The behavior of Nb-Ta-bearing ilmenorutile in aqueous fluid at high pressures and temperature	August 3-6, 2012
Y. Song	University of Western Ontario	High-pressure study of ZnO nanowires	August 5-7, 2012
K. Glazyrin L. Miyagi	Yale University Montana State University – Bozeman	High-pressure room-temperature behavior of heavy ion beam irradiated graphite	August 8-10, 2012
R. Saavedra	LANL	Electrical resistance measurements at high pressure	August 8-11, 2012
M. Lipp	LLNL	Cerium ultrasound under high pressure and temperature	August 8-12, 2012
J. Jeffries	LLNL	Magnetic moments in (Ca,Sr)Fe_2As_2 under pressure	August 8-13, 2012
A. Campbell D. Heinz R. Fischer M. Valdez	University of Chicago Washington University in St. Louis	High pressure XRD of iron alloys	August 10-12, 2012
K. Catalli	LLNL	DAC Pu experiments	August 11-14, 2012
H. Cynn	LLNL	5f metal compression at high pressure and high temperature	August 11-14, 2012
M. Armentrout	University of California – Los Angeles	XRD study of metals under high pressure	August 12-14, 2012
Y. Kono	HPCAT	Developments in Paris-Edinburgh cells	August 12-16, 2012

S. Dorfman	Ecole Polytechnique Federale de Lausanne, Switzerland	Spin states of iron in $(Fe_{0.75}Al_{0.25})(Al_{0.25}Si_{0.75})O_3$ perovskite and glass	August 13-17, 2012
M. Somayazulu	Carnegie	Synthesis of Xe-C and Xe-Cl_2 compounds at high *P-T* conditions	August 15-17, 2012
F. Yang	Stanford University	Diamondoids under high pressure	August 17-19, 2012
B. Li	HPSynC	High pressure study of Cr	August 17-19, 2012
Z. Yu	Harbin Institute of Technology	High pressure XRD study of NiP	August 17-19
L. Zhang	Carnegie	Physical properties of mantle silicates at high pressure	August 17-19, 2012
C. Li	Harbin Institute of Technology	XRD study on nlip	August 17-20, 2012
B. Mattern	University of Washington	XES of Nd	August 17-21, 2012
L. Kong	Harbin Institute of Technology	High pressure study of the Pb-based relaxors near MPB	August 19-20, 2012
M. Frank	Northern Illinois University	An experimental study of the Mg_2SiO_4-CO_2 system	August 19-21, 2012
H. Scott	Indiana University – South Bend	An examination of the $MgSiO_3$-MgO-CO_2 system at high pressures and temperatures	August 19-21, 2012
G. Shen Y. Meng R. Boehler A. Karandikar	HPCAT Carnegie	Pulse laser heating of metals	August 21-23, 2012
M. Guthrie	Carnegie	XRD of water at high pressure	August 21-23, 2012
B. Lavina K. Kothapali	University of Nevada – Las Vegas	Stability of Fe_4O_5 at high pressure and high temperature	October 3-5, 2012
L. Kong G. Liu	Carnegie Pennsylvania State University	X-ray white Laue diffraction on single crystals under high pressure	October 3-6, 2012
D. Ikuta	Carnegie	Single crystal XRD at high pressures	October 4-6, 2012
L. Zhang	Carnegie	Physical properties of silicates at high pressure and temperature	October 5-7, 2012
B. Li	HPSynC	High pressure study of IR	October 5-7, 2012
E. Boulard	Stanford University	Enstatite calcite	October 5-7, 2012
A. Gleason M. Reagan	Stanford University	Magnetic properties of FeOOH under pressure	October 5-8, 2012
J. Lim Y. Lee D. H. Seoung Y. Lee	Yonsei University	Carbons in nanopores	October 6-8, 2012
J. Wu	University of Texas – Austin	Phase stability and melting curve of the Fe-C alloys in the Earth's core	October 7-11, 2012
J. Baker S. V. Raju R. Kumar	University of Nevada – Las Vegas	High pressure inelastic x-ray scattering studies on Yb systems	October 10-12, 2012
Y. Song L. Zhou A. Zhao	University of Western Onatario	Structural investigation of titanium dioxide nanotubes at high pressure	October 10-13, 2012

T. Strobel	Carnegie	Carbon compounds with Mg	October 11-13, 2012
T. Yu	University of Chicago	Sodium silicate glass/liquid structure measurement	October 11-13, 2012
D. Antonio F. Nasreen	University of Nevada – Las Vegas	Low temperature, high pressure RIXS on YbCu Ga	October 12-14, 2012
Y. Shi	Stanford University	High pressure constraints on Earth core formation	October 13-14, 2012
Z. Zeng Q. Zeng	Stanford University	Li-Si alloy studies	October 13-14, 2012
Y. Wang I. Efthymiopoulos	Oakland University	Spinels under high pressure	October 13-15, 2012
A. Kavner D. Hummer S. Palaich	University of California – Los Angeles	High pressure behavior of carbonate-silicate melts	October 13-15, 2012
B. Li	HPSynC	High pressure XRD of Ir	October 13-15, 2012
Y. Shi	Stanford University	High *P-T* study of silicate and iron sulfate	October 13-15, 2012
L. Zhang	Carnegie	Physical properties of silicates at high pressure and high temperature	October 13-15, 2012
P. Dera	University of Chicago	High-pressure single-crystal x-ray microdiffraction investigation of s-triazine derivatives	October 15-18, 2012
C. Park J. Smith	Carnegie	External heavy heating	October 15-19, 2012
H. Cynn	LLNL	Heavy heating coupled with non-contact temperature measurements	October 15-19, 2012
Z. Jenei	LLNL	White beam radiography	October 17-19, 2012
C. Holl	Princeton University	Compression of alumina to 2 Mbar	October 18-20, 2012
B. Chen J. Liu Z. Li	University of Michigan	Magnetic transition of Fe_7C_3 up to 1 Mbar by XES	October 19-21, 2012
G. Tsoi W. Uhoya	University of Alabama – Birmingham	High pressure effects on iron based compounds	October 19-22, 2012
B. Chen	University of Michigan	XES study on pressure induced spin transitions of Fe_7C_3	October 21-22, 2012
L. Bai	University of Nevada – Las Vegas	Pressure-induced spin transition in $PbCrO_3$	October 21-22, 2012
Z. Zhao W. Yang	HPCAT HPSynC	High pressure melting of SiGe	October 21-26, 2012
Q. Li D. Zhou	University of Nevada – Las Vegas	High pressure XRD of SnSe	October 22-23, 2012
S. Haravifard	University of Chicago	SCBO under pressure	October 22-25, 2012
X. Lu	University of Nevada – Las Vegas	XRD study of Nb-doped TiO_2	October 24-25, 2012
G. Borstard H. Y. Chang	Washington State University	High pressure XRD of simple binary mixtures	October 24-26, 2012
K. Kothapali F. Nasreen	University of Nevada – Las Vegas	Valency of $CeFe_4P_{12}$ and $Ce_{0.5}La_{0.5}Fe_4P_{12}$ under pressure	October 24-26, 2012
J. Wu J. Zhu	Chinese Academy of Sciences LANL	Single crystal diffraction of $SrIrO_3$, Sr_2IrO_4, $LiAlSiO_4$ under high pressure	October 25-29, 2012

B. Li	HPSynC	High pressure study of Ir	October 26-28, 2012
L. Zhang	Carnegie	Physical properties of silicates at high pressure and temperature	October 26-28, 2012
Z. Zhao	HPCAT	Structures of glass carbon under pressure	October 26-28, 2012
Y. Shi	Stanford University	Fe-Mg partitioning at ultrahigh pressure in perovskite and post-perovskite	October 26-28, 2012
C. Park H. Yan	HPSynC	Reflectivity study of high *P-T* mineral fluid interface	October 26-29, 2012
K. Kothapalli B. Lavina	University of Nevada – Las Vegas	HIgh Pressure XRD studies $CeFe_4P_{12}$ and $Ce_{0.5}La_{0.5}Fe_4P_{12}$	October 31-November 2, 2012
Devon Mortensen M. Lipp	University of Washington	f-electron delocalization	October 31-November 4, 2012
J. Pigott	Ohio State University	Equations of state and melting curves of Pt, PtC, Fe, Ni, MgO, Al_2O_3, and SiO_2 to 100 GPa and 5500 K using controlled geometry	November 1-3, 2012
D. Reaman	University of Chicago	Equations of state of nanofabricated samples	November 1-3, 2012
M. Somayazulu	Carnegie	Xe chemistry under high pressure	November 3-4, 2012
M. Pravica N. Rondeau L. Bai	University of Nevada – Las Vegas	Studies in hard x-ray induced chemistry	November 3-6, 2012
J. Liu M. Lang F. Zhang	University of Michigan	Formation of magnesite from forsterite and CO_2 at mantle conditions at depths greater than 150 km	November 4-6, 2012
Y. Ding	ANL	High-pressure Hg L23 PYF XAS	November 4-7, 2012
S. Wang	Stanford University	XANES on Hg-based cuprate at high pressure	November 4-8, 2012
D. Ikuta	HPCAT	Single crystal XRD at high pressures	November 7-9, 2012
S. MacLeod	Atomic Weapons Establishment, UK	Melting of Ti at high pressure	November 7-9, 2012
H. Cynn	LLNL	Measuring photo-diode response coupled with thermal radiation during laser heating at high pressure	November 7-9, 2012
C. Sanloup C. deGrouchy J. Drewitt H. Spice	University of Edinburgh	Effect of high pressure and fO_2 on the viscosity of molten fayalite	November 8-12, 2012
J. Jeffries	LLNL	Fe local moments in the collapsed tetragonal phase of $(Ca,Sr)Fe_2As_2$	November 8-12, 2012
Y. Shi	Stanford University	High PT study of silicates, Fe, and FeS	November 9-10, 2012
K. Catalli J. H. Klepeis	LLNL	EOS of uranium compounds	November 9-12, 2012
J. Cheng	APS	Fe-Mg partitioning at ultrahigh pressure in perovskite and post-perovskite	November 10-12, 2012
J. Wang B. Li	HPSynC	High pressure study of tungsten	November 10-11, 2012
C. Liu	Harbin Institute of Technology	High pressure and low temperature phase diagram mapping	November 14-16, 2012
R. Li L. L. Li	Harbin Institute of Technology	Structural evolution of powder crystal at high pressure	November 14-17, 2012

J. Cheng	APS	Fe-Mg partitioning at ultrahigh pressure in perovskite and post-perovskite	November 15-19, 2012
Q. Zeng Z. Zeng	Stanford University	Volume of metallic glass under high pressure	November 16-20, 2012
N. Velisavljevic R. Chellappa R. Saavedra	LANL	High compression rate experiments	November 16-18, 2012
Z. Zhao W. P. Hsieh	Stanford University	High pressure and temperature study on VO_2	November 17-20, 2012
F. Nasreen D. Antonio	University of Nevada – Las Vegas	High pressure XANES and XRD of U_2Zn_{17} and UCd_{11} compounds	November 20-21, 2012
M. Pravica L. Bai	University of Nevada – Las Vegas	Studies of hydrazine and boric acid at high pressure	November 20-21, 2012
Z. Zhao	HPCAT	The phase transition of glass carbon under pressure	November 20-22, 2012
K. Kothapalli	University of Nevada – Las Vegas	NSF studies on Fe_4O_5	November 21-22, 2012
X. Chen	HPSynC	Spin-phonon coupling in spinels	November 23-24, 2012
E. Zepeda-Alarcon P. Kaercher	University of California – Berkeley	Deformation and phase transformations of SiO_2 at high pressure and temperature	November 23-25, 2012
J. B. Zhang L. Liu Y. Peng	HPSynC	High pressure powder diffraction of Bi2223	November 23-25, 2012
V. Struzhkin	Carnegie	Spin and valence states of iron containing Earth minerals	November 23-26, 2012
J. Howard	University of Nevada – Las Vegas	XRD of lithium rich anti-perovskites under high pressure and medium temperature	November 25-26, 2012
M. Ahart	Carnegie	Pressure induced transitions in ferroelectric $Pb(Zr_{0.48}Ti_{0.52})O_3$ single crystals	November 25-27, 2012
N. Velisavljevic	LANL	Development of electrical and thermal measurements with Paris-Edinburgh cell	November 25-30, 2012
J. Baker R. Kumar	University of Nevada – Las Vegas	Thermal conductivity measurements with Paris-Edinburgh cell	November 25-December 1, 2012
H. R. Wenk	University of California – Berkeley	Rheology in the Earth's mantle: Deformation of silicate perovskite and magnesiowuestite	November 27-28, 2012
H. Cynn S. MacLeod	LLNL Atomic Weapons Establishment, UK	5f metals at high pressure and high temperature	November 28-December 1, 2012
D. Ikuta	HPCAT	Single crystal XRD at high pressures and high temperatures	November 28-December 4, 2012
Q. Zeng Z. Zeng	Stanford University	Power-law scaling of density in metallic glass under high pressure	November 29-30, 2012
J. Wu S. Feng	University of Texas – Austin Chinese Academy of Science	XES of $SrFe_2As_2$ under high pressure and low temperature	November 30-December 4, 2012
D. Antonio	University of Nevada – Las Vegas	XRD of Re_2W_3 and Re_2Mo_3	December 1-3, 2012
R. Kumar	University of Nevada – Las Vegas	Low temperature high pressure XRD studies on iron pnictides and strongly correlated electron systems	December 1-3, 2012
L. Bai	University of Nevada – Las Vegas	Energy dependent studies of radiation induced decompression	December 1-4, 2012
M. Pravica	University of Nevada – Las Vegas	High pressure and radiation-induced studies of urea	December 1-4, 2012

P. Bowden R. Chellappa	LANL	High pressure studies on energetic materials and polymers	December 3-7, 2012
H. Cynn	LLNL	Angle-dispersive XRD of uranium sulfide at cryogenic temperatures	December 5-7, 2012
D. Yu Y. Shu	Yanshan University	Structural transformation and microstructure heritable of pure bismuth	December 5-8, 2012
Z. Zhao	HPCAT	Phase transition of Bi under high pressure and high temperature	December 5-8, 2012
K. Catalli	LLNL	XES on actinides	December 5-11, 2012
E. Bauer	LANL	XES on Du and Pu samples	December 5-11, 2012
Y. Y. Chang J. Lazars X. Liu	Northwestern University	Compressibility of BCN to 100 GPa	December 7-9, 2012
C. Tracy S. Park A. Cusick	University of Michigan	Investigation of actinide oxides to high-energy irradiation	December 7-10, 2012
Z. Jenei	LLNL	Ultrasonic velocity measurement of Ce in PEC	December 8-11, 2012
N. Velisavljevic	LANL	RAD sample at high pressure	December 10-13, 2012
L. Bai	University of Nevada – Las Vegas	RXES of selenides	December 12-14, 2012
H. Cynn W. Evans	LLNL	Compression behavior of 5f metal compounds at high temperature	December 12-15, 2012
L. Bai M. Pravica	University of Nevada – Las Vegas	Energy dependent studies of x-ray induced decomposition chlorate salts	December 13-15, 2012
J. Jeffries	LLNL	Low-temperature compression of $(Ca,Sr)Fe_2As_2$ through the volume collapse	December 15-16, 2012
Q. Smith	University of Nevada – Las Vegas	$KClO_3$ decomposition	December 15-16, 2012
J. Cheng B. Li	HPSynC	High pressure study of FeO, Re, Pt, and W	December 15-17, 2012
L. Zhang	Carnegie	Physical properties of silicates at high pressure	December 15-17, 2012
M. Reagan	Stanford University	Spin transitions of FeOOH	December 16-18, 2012
D. Popov	HPCAT	Development of Laue technique	December 16-19, 2012
R. Barabash	ORNL	High pressure induced displacive transformations in shape-memory alloys	December 16-19, 2012
L. Liu	HPSynC	The powder XRD of polycrystalline under high pressure with DAC	December 17-18, 2012
Y. Sun Y. Lee D. Seoung	Florida International University	Rehydrogenation and phase transition of ammonia borane	December 17-19, 2012
J. Cheng	HPSynC	High pressure study of boron nitride	December 18-19, 2012
Y. Gao	Texas Tech University	Rotation, diffraction, spectroscopy	December 18-19, 2012
T. Gu	Carnegie	XES of Fe_3CS, P_7	December 18-19, 2012

B. U2A Infrared Beamline (NSLS)

Beamline U2A is managed by **Carnegie** and provides useful materials characterization capabilities not available at other beamlines. The principal source of support for this beamline is the National Science Foundation, through the EAR COMPRES consortium. CDAC has a 20% membership in the facility by virtue of **Carnegie** management. CDAC provided partial salary support for Beamline scientist **Zhenxian Liu** as well as beamline upgrades and supplies.

User Name	Affiliations	Project	Dates
H. Feng	Montclair State University	Examination of organic contaminants (PAHs) in passaic river sediments using synchrotron-UV-FTIR techniques	January 11-12, 2011
Y. J. Lee D. Liu D. Seoung Y. M. Lee	Yonsei University	High-pressure powder diffraction ftudies of zeolites	January 19-24, 2011
X. Wang	BNL	*In situ* and *ex situ* x-ray absorption spectroscopic on $LiFe_yMn_{1-y}PO_4$ cathode materials for high-power lithium-ion batteries	January 31-February 2, 2011
W. Han	BNL	Study gas storage in boron nitride nanostructures by high-pressure IR and Raman	February 9-11, 2011
M. Lang F. Zhang	University of Michigan	Phase transitions in minerals induced by ion beams and high pressure: A novel approach in geosciences	February 15-17, 2011
K. Adams	Northwestern University	Low temperature visible to near-IR reflectivity of ethane-methane mixtures with applications to hydrocarbon lakes on Titan	February 21-26, 2011
C. S. Zha	Carnegie	IR study for dense hydrogen under wide simultaneous *P-T* conditions	February 27-March 3, 2011
M. Pravica M. Galley	University of Nevada – Las Vegas	High pressure mid-IR studies of melamine	March 18-20, 2011
B. Liu Q. Li D. Liu	Jilin University	Pressure-induced amorphization and polyamorphism in TiO_2 nanomaterials	March 21-23, 2011
H. Feng	Montclair State University	Examination of organic contaminants (PAHs) in passaic river sediments using synchrotron-UV-FTIR techniques	March 24-25, 2011
E. Hausrath	University of Nevada – Las Vegas	Characterization of fumarolic alterations and implications for Mars	April 1-3, 2011
P. Gao T. Tyson	New Jersey Institute of Technology	Spin-driven local distortions in multiferroic hexagonal $ReMnO_3$: IR measurements	April 4-8, 2011
C. S. Zha	Carnegie	IR study for dense hydrogen under wide simultaneous *P-T* conditions	April 13-14, 2011
N. Velisavljevic	LANL	IR measurement of FOX-7 reacton and detonation products	April 21-23, 2011
J. Musfeldt	University of Tennessee	Pressure-induced switching of the Jahn-Teller axis in $Cu(pyz)F_2(H_2O)_2$ by synchrotron IR spectroscopy	April 25-29, 2011
C. Zha	Carnegie	IR study for dense hydrogen under wide simultaneous *P-T* conditions	May 21-22, 2011
H. Feng	Montclair State University	Examination of organic contaminants (PAHs) in passaic river sediments using synchrotron-UV-FTIR techniques	June 1-3, 2011

Y. J. Lee D. Liu D. Seoung Y. M. Lee	Yonsei University	High-pressure powder diffraction studies of zeolites	June 6-12, 2011
G. Amulele K. Otsuka	Yale University	*In situ* FTIR measurements on hydrogen solubility and speciation in olivine and magnesiowüstite at high pressures and temperatures	June 27-30, 2011
C. S. Zha	Carnegie	IR study for dense hydrogen under wide simultaneous *P-T* conditions	September 1-2, 2011
P. Gao T. Wu T. Tyson	New Jersey Institute of Technology	High pressure IR and XRD studies of multiferroic orthorhombic $REMnO_3$	September 6-10, 2011
C. S. Zha	Carnegie	IR study for dense hydrogen under wide simultaneous *P-T* conditions	September 14-16, 2011
M. Pravica Y. Liu	University of Nevada – Las Vegas	Studies of MnO_2 and $KClO_3$ under extreme conditions	September 16-19, 2011
C. S. Zha	Carnegie	IR study for dense hydrogen under wide simultaneous *P-T* conditions	September 22-23, 2011
G. Yang	BNL	Synchrotron IR microspectroscopy, Raman spectroscopy and photoluminescence spectroscopy investigation of CdZnTe and CdMnTe crystals	September 28-30, 2011
N. Velisavljevic R. Chellappa	LANL	IR measurement of FOX-7 reacton and detonation products	October 5-8, 2011
C. S. Zha	Carnegie	IR study for dense hydrogen under wide simultaneous *P-T* conditions	October 9-13, 2011
H. Feng	Montclair State University	Examination of organic contaminants (PAHs) in passaic river sediments using synchrotron-UV-FTIR techniques	October 26-28, 2011
G. Yang	BNL	Synchrotron IR microspectroscopy, Raman spectroscopy and photoluminescence spectroscopy investigation of CdZnTe and CdMnTe crystals	October 30, 2011
J. Chen Y. Sun	Florida International University	Synchrotron IR spectroscopy of ammonia borane in metal-organic frameworks.	October 31, 2011
J. Tse	University of Saskatchewan	Pressure induced magetic and insulator to metal transitions in nano-organometallic radical complexes	November 1-6, 2011
C. S. Zha	Carnegie	IR study for dense hydrogen under wide simultaneous *P-T* conditions	November 9-13, 2011
Q. Li R. Liu	Jilin University	Pressure induced metal-insulator transition in VO_2 bulks and nanomaterials	November 14-17, 2011
M. Lang F. Zhang S. Botis	University of Michigan	Phase transitions in minerals induced by ion beams and high pressure: A novel approach in geosciences	November 18-22, 2011
Y. Hu Y. Song	University of Western Ontario	High pressure studies of ZIF materials by IR spectroscopy	December 14-19, 2011
M. Aihaiti	Carnegie	The pressure dependence of hydrogen vibron at 300 K	January 15, 2012
C. S. Zha	Carnegie	IR study for dense hydrogen under wide simultaneous *P-T* conditions	January 23, January 25-26, 2012
M. Aihaiti	Carnegie	The pressure dependence of hydrogen vibron at 300 K	January 24, 2012

C. S. Zha	Carnegie	IR study for dense hydrogen under wide simultaneous *P-T* conditions	January 25-26, 2012
J. C. Jenkins	Army Research Laboratory	High pressure IR characterization of extended solids: Carbon monoxide	February 8-10, 2012
Y. J. Lee T. Kim D. Seoung Y. M. Lee	Yonsei University	High pressure powder diffraction studies of zeolites	February 13-16, 2012
G. Yang	BNL	Synchrotron IR microspectroscopy, Raman spectroscopy and photoluminescence spectroscopy investigation of CdZnTe and CdMnTe crystals	February 21-23, 2012
C. S. Zha	Carnegie	IR study for dense hydrogen under wide simultaneous *P-T* conditions	March 8-9, 2012
M. Pravica Y. Liu	University of Nevada – Las Vegas	Studies of MnO_2 and $KClO_3$ under extreme conditions	March 10-12, 2012
H. Feng	Montclair State University	Examination of metal chelation on functionalized graphene surface for development of metal catalysts and sensors	March 13-15, 2012
J. Musfeldt S. Rostom	University of Tennessee	Pressure-induced switching of the Jahn-Teller axis in $Cu(pyz)F_2(H_2O)_2$ by synchrotron IR spectroscopy	March 18-25, 2012
M. Lang F. Zhang S. Botis	University of Michigan	Response of minerals to extreme conditions of ion irradiation and high pressure: A novel approach in geosciences	March 25-28, 2012
J. Girard	Florida International University	IR studies of water incorporation in San Carlos olivine	March 28, 2012
Q. Li R. Liu	Jilin University	Pressure induced metal-insulator transition in VO_2 bulks and nanomaterials	March 28-31, 2012
T. Yu T. Wu T. Tyson	New Jersey Institute of Technology	Electronically driven ferroelectricity in $REMnO_3$	April 4-7, 2012
R. Chellappa P. Bowden J. Vita N. Mack F. Rein D. Dattelbaum	LANL	Role of mode anharmonicity in initiation of high explosives	April 9-10, 2012
R. Chellappa P. Bowden J. Vita N. Mack F. Rein D. Dattelbaum	LANL	High pressure chemistry of simple organics	April 11-16, 2012
C. Unterborn	Ohio State University	Hydrogen and carbon incorporation mechanisms in deep Earth minerals	April 19-22, 2012
C. S. Zha	Carnegie	IR study for dense hydrogen under wide simultaneous *P-T* conditions	April 23-25, 2012
J. Townsend	Northwestern University	Water in post-perovskite: A hydrogen trap at the core-mantle boundary?	April 26-29, 2012
C. S. Zha	Carnegie	IR study for dense hydrogen under wide simultaneous *P-T* conditions	June 2-4, 2012

J. Chen Y. Sun S. Huang S. Najiba	Florida International University	IR spectroscopy of boron at high pressures	June 7-11, 2012
B.Grocholski E. Stevenson	Smithsonian National Museum of Natural History	Water storage capacity of lower mantle perovskite and stishovite	June 11-13, 2012
V. Struzhkin A. Gavrilyuk	Carnegie	Reflectivity spectra of simple transition metal oxides at multinmegabar pressures	June 14-17, 2012
C. Ma	Jilin University	The behavior of hydrogen bond under extreme conditions in typical linear or cyclic organic compounds under extreme conditions	June 18-19, 21-28, 2012
J. Chen	Florida International University	IR spectroscopy of boron at high pressures	June 29-30, 2012
C. Ma	Jilin University	The behavior of hydrogen bond under extreme conditions in typical linear or cyclic organic compounds under extreme conditions	July 1-2, 5-9, 2012
Q. Li R. Liu	Jilin University	Pressure induced metal-insulator transition in VO_2 bulks and nanomaterials	July 10-13, 2012
C. Ma	Jilin University	The behavior of hydrogen bond under extreme conditions in typical linear or cyclic organic compounds under extreme conditions	July 14-19, 2012
R. Chellappa V. Manner F. Rein	LANL	High pressure chemistry of simple organics	July 20-27, 2012
X. Huang F. Huang	Jilin University	*In situ* high-pressure study of heterocycles by IR spectroscopy	July 28-August 1, 2012
W. Panero	Ohio State University	Hydrogen and carbon incorporation mechanisms in deep Earth minerals	August 2-4, 2012
C. S. Zha	Carnegie	IR study for dense hydrogen under wide simultaneous *P-T* conditions	August 5-11, 2012
X. Cheng	Zhengzhou University of Light Industry	A phase transformation of ionic liquid [BMIM][PF6] under high pressure	September 13-20, 2012
Z. Liu C. Ma	Carnegie Jilin University	The Behavior of hydrogen bond under extreme conditions in typical linear or cyclic organic compounds under extreme conditions	September 20-25, 27, 2012
X. Xi	Brookhaven National Laboratory	Evolution of superconductivity with pressure in iron-based superconductors studied by IR spectroscopy	September 28, 2012
Z. Liu C. Ma	Carnegie Jilin University	The behavior of hydrogen bond under extreme conditions in typical linear or cyclic organic compounds under extreme conditions	September 29-30, 2012
Y. Sun S. Huang S. Najiba	Florida International University	IR spectroscopy of boron at high pressures	October 1-5, 2012
Q. Cui C. Ma	Jilin University	The behavior of oxide compounds under extreme conditions	October 6-12, 2012

Z. Liu C. Ma	Carnegie Jilin University	The Behavior of hydrogen bond under extreme conditions in typical linear or cyclic organic compounds under extreme conditions	October 18-20, 24-27, 2012
J. Musfeldt K. O'Neal T. Brinzari	University of Tennessee	Pressure-induced switching of the Jahn-Teller axis in $Cu(pyz)F_2(H_2O)_2$ by synchrotron IR spectroscopy	October 29-November 3, 2012
B.Grocholski E. Stevenson	National Museum of Natural History	Water storage capacity of lower mantle perovskite and stishovite	November 3-6, 2012
W. Panero J. Pigott	Ohio State University	Hydrogen and carbon incorporation mechanisms in deep Earth minerals	November 7, 2012
Z. Liu M. Ahart	Carnegie	IR study for dense hydrogen under wide simultaneous *P-T* conditions	November 8-10, 2012
V. Struzhkin	Carnegie	The pressure dependence of hydrogen vibron at 300 K	November 14-16, 2012
E. Boulard	Stanford University	An IR study of carbon environments in new high-pressure carbonates phases	November 18-20, 2012
Z. Liu M. Ahart	Carnegie	IR study for dense hydrogen under wide simultaneous *P-T* conditions	November 20-21, 2012

References

1. Rhodes, R., *The Making of the Atomic Bomb* (Simon and Schuster, New York, 1986).
2. Yoder Jr., H. S., *Centenial History of the Carnegie Institution of Washington: The Geophysical Laboraory* (Cambridge University Press, New York, 2004).
3. Munoz, J. A., M. S. Lucas, O. Delaire, M. Winterrose, L. Mauger, C. W. Li, A. O. Sheets, M. B. Stone, D. L. Abernathy, Y. Xiao, P. Chow, and B. Fultz, Positive vibrational entropy of chemical ordering in FeV, *Phys. Rev. Lett.* **107**, 115501 (2011).
4. McWilliams, R. S., D. K. Spaulding, J. H. Eggert, P. M. Celliers, D. G. Hicks, R. F. Smith, G. W. Collins, and R. Jeanloz, Phase transformations and metallization of magnesium oxide at high pressure and temperature, *Science* **338**, 1330-1333 (2012).
5. Vailionis, A., E. G. Gamaly, V. Mizeikis, W. Yang, A. V. Rode, and S. Juodkazis, Evidence of superdense aluminum synthesized by ultrafast microexplosion, *Nature Comms.* **2**, 445 (2011).
6. Zha, C. S., Z. Liu, and R. J. Hemley, Synchrotron infrared measurements of dense hydrogen to 360 GPa, *Phys. Rev. Lett.* **108**, 146402 (2012).
7. Benjamin, A. S., M. Ahart, S. A. Gramsch, L. L. Stevens, E. B. Orler, D. M. Dattelbaum, and R. J. Hemley, Acoustic properties of Kel F-800 copolymer up to 85 GPa, *J. Chem. Phys.* **137**, 014514 (2012).
8. Dias, R. P., C. S. Yoo, M. Kim, and J. Tse, Insulator-metal transition of highly compressed carbon disulfide, *Phys. Rev. B* **84**, 144104 (2011).
9. Jeffries, J. R., N. P. Butch, K. Kirshenbaum, S. R. Saha, G. K. Samudrala, S. T. Weir, Y. K. Vohra, and J. Paglione, Suppression of magnetism and developmetn of superconductivity within the collapsed tetragonal phase of $Ca_{0.67}Sr_{0.33}Fe_2As_2$ under pressure, *Phys. Rev. B* **85**, 184501 (2012).
10. Chen, B., K. Lutker, S. V. Raju, J. Yan, J. Kanitpanyacharoen, J. Lei, S. Yang, H. R. Wenk, H. K. Mao, and Q. Williams, Pressure-promoted texturing in nanocrystalline nickle: Probing the lower size limit of dislocation activity, *Science* **338**, 1448-1451 (2012).
11. Shen, G., D. Ikuta, S. V. Sinogeikin, Q. Li, Y. Zhang, and C. Chen, Direct observation of a pressure-induced precursor lattice in silicon, *Phys. Rev. Lett.* **109**, 205503 (2012).
12. Xu, M., Y. Q. Cheng, L. Wang, H. W. Sheng, Y. Meng, W. G. Yang, X. D. Han, and E. Ma, Pressure tunes electrical resistivity by four orders of magnitude in amorphous $Ge_2Sb_2Te_5$ phase-change memory alloy, *Proc. Nat. Acad. Sci.* **109**, E1055-E1062 (2012).
13. Mao, W. L., H. K. Mao, P. Eng, T. P. Trainor, M. Newville, C. C. Kao, D. L. Heinz, J. Shu, Y. Meng, and R. J. Hemley, Bonding changes in compressed superhard graphite, *Science* **302**, 425-427 (2003).
14. Umemoto, K., R. M. Wentzcovitch, S. Saito, and T. Miyake, Body-centered tetragonal C_4: A viable sp^3 carbon allotrope, *Phys. Rev. Lett.* **104**, 125504 (2010).
15. Zhou, X. F., G. R. Qian, X. Dong, L. Zhang, Y. Tian, and H. T. Wang, Ab initio study of the formation of transparent carbon under pressure, *Phys. Rev. B* **82**, 134126 (2010).
16. Li, Q., Y. Ma, A. R. Oganov, H. Wang, H. Wang, Y. Xu, T. Cui, H. K. Mao, and G. Zhou, Superhard monoclinic polymorph of carbon, *Phys. Rev. Lett.* **102**, 175506 (2009).
17. Wang, Y., J. E. Panzik, B. Kiefer, and K. K. M. Lee, Crystal structure of graphite under room-temperature compression and decompression, *Sci. Reports* **2**, 520 (2012).
18. Lin, Y., L. Zhang, H. K. Mao, P. Chow, Y. Xiao, M. Baldini, J. Shu, and W. L. Mao, Amorphous diamond - A high-pressure superhard carbon allotrope, *Phys. Rev. Lett.* **107**, 175504 (2011).
19. Wang, L., W. Yang, Y. Xiao, B. Liu, P. Chow, G. Shen, and H. K. Mao, Application of a new composite c-BN gasket assembly for high pressure IXS studies of carbon related materials, *Rev. Sci. Instrum.* **82**, 073902 (2011).
20. Wang, L., Y. Ding, U. Patel, W. Yang, Z. Xiao, Z. Cai, W. L. Mao, and H. K. Mao, Studying single nanocrystals under high pressure using an x-ray nanoprobe, *Rev. Sci. Instrum.* **82**, 043903 (2011).
21. Subramanian, N., A. F. Goncharov, V. V. Struzhkin, M. Somayazulu, and R. J. Hemley, Bonding changes in hot fluid hydrogen at megabar pressures, *Proc. Nat. Acad. Sci.* **108**, 6014 (2011).
22. Chen, X. J., C. Zhang, Y. Meng, R. Q. Zhang, H. Q. LIn, V. V. Struzhkin, and H. K. Mao, β-tin->Imma->sh phase transition of germanium, *Phys. Rev. Lett.* **106**, 135502 (2011).
23. Xie, M., R. Mohammadi, Z. Mao, M. M. Armentrout, A. Kavner, R. B. Kaner, and S. H. Tolbert, Exploring the high-pressure behavior of superhard tungsten tetraboride, *Phys. Rev. B* **85**, 064118 (2012).
24. Dorfman, S. M., F. Jiang, Z. Mao, A. Kubo, Y. Meng, V. Prakapenka, and T. S. Duffy, Phase transitions and equation of state of alkaline earth flourides CaF_2, SrF_2, and BaF_2 to Mbar pressures, *Phys. Rev. B* **81**, 174121 (2010).
25. Haines, J., J. M. Leger, and O. Schulte, High-pressure isosymmetric phase transition in orthorhombic lead fluoride, *Phys. Rev. B* **57**, 7551-7555 (1998).

26. Dera, P., B. Lavina, L. A. Borkowski, V. B. Prakapenka, S. R. Sutton, M. L. Rivers, R. T. Downs, N. Z. Boctor, and C. Prewitt, High-pressure polymorphism of Fe_2P and its implications for meteorites and Earth's core, *Geophys. Res. Lett.* **35**, L10301 (2008).
27. Lang, M., J. Lian, J. M. Zhang, F. X. Zhang, W. J. Weber, C. Trautmann, and R. C. Ewing, Single-ion tracks in $Gd_2Zr_{2-x}Ti_xO_7$ pyrochlores irradiated with swift heavy ions, *Phys. Rev. B* **79**, 224105 (2009).
28. Zhang, J. M., M. Lang, M. D. Toulemonde, R., R. C. Ewing, and W. J. Weber, Nanoscale phase-transitions under extreme conditions within an ion track, *J. Mater. Res.* **25**, 1344-1351 (2008).
29. Zhang, F. X., J. W. Wang, J. Lian, M. Lang, and U. Becker, Phase stability and pressure dependence of deffect formation in $Gd_2Ti_2O_7$ and $Gd_2Zr_2O_7$ pyrochlores, *Phys. Rev. Lett.* **100**, 045503 (2008).
30. Zhang, F. X., M. Lang, Z. X. Liu, and R. C. Ewing, Pressure-induced dissordering and anamlous lattice expansion in $La_2Zr_2O_7$ pyrochlore, *Phys. Rev. Lett.* **105**, 015503 (2010).
31. Lang, M., F. X. Zhang, J. Zhang, J. Wang, B. Schuster, C. Trautmann, R. Neumann, U. Becker, and R. C. Ewing, Nanoscale manipulation of the properties of solids at high pressure with relativistic heavy ions, *Nature Mat.* **8**, 793-797 (2009).
32. Xia, H., G. Parthasarathy, H. Luo, Y. K. Vohra, and A. L. Ruoff, Crystal structures of group IVa metals at ultrahigh pressures, *Phys. Rev. B* **42**, 6736-6738 (1990).
33. Errandonea, D., Y. Meng, M. Somayazulu, and D. Häusermann, Pressure-induced alpha -> omega transition in titanium metal: a systematic study of the effects of uniaxial stress, *Physica B* **355**, 116-125 (2005).
34. Vohra, Y. K., S. K. Sikka, S. N. Vaidya, and R. Chidambaram, Impurity effects and reaction kinetics of the pressure-induced $\alpha \rightarrow \omega$ transformation in Ti *J. Phys. Chem. Solids* **38**, 1293-1296 (1977).
35. Velisavljevic, N., G. N. Chesnut, L. L. Stevens, and D. M. Dattelbaum, Effects of interstitial impurities on the high pressure martensitic α to ω structural transformation and grain growth in zirconium, *J. Phys.: Cond. Matt.* **23**, 125402 (2011).
36. Bos, J. W. G., Structures and thermoelectric properties of the infinitely addaptive series $(Bi_2)_m(Bi_2Te_3)_n$, *Phys. Rev. B* **75**, 195203 (2007).
37. Jeffries, J. R., A. L. LIma Sharma, P. A. Sharma, C. D. Spataru, K. McCall, J. D. Sugar, S. T. Weir, and Y. K. Vohra, Distinct supercondicting states in the pressure-induced metallic structures of the nominal semimental Bi_4Te_3, *Phys. Rev. B* **84**, 092505 (2011).
38. Wang, L., B. Liu, H. Li, W. Yang, Y. Ding, S. V. Sinogeikin, Y. Meng, Z. Liu, X. Zeng, and W. L. Mao, Long-range ordered amorphous carbon clusters: A crystalline material with amorphous building blocks, *Science* **337**, 825-828 (2012).
39. Dewale, A., M. Torrent, P. Loubeyre, and M. Mezouar, Compression curves of transition metals in the Mbar range: Experiments and projector augmented-wave calculations, *Phys. Rev. B* **78**, 104102 (2008).
40. Sata, N., G. Shen, M. L. Rivers, and S. R. Sutton, Pressure-volume equation of state of the high-pressure B2 phase of NaCl, *Phys. Rev. B* **65**, 104114 (2002).
41. Ono, S., T. Kikegawa, and Y. Ohishi, Structural property of CsCl-type sodium chloride under pressure, *Solid State Comm.* **137**, 514-521 (2006).
42. Hirose, K., R. Sinmyo, N. Sata, and Y. Ohishi, Determination of post-perovskite phase transition boundary in Mg-SiO_2 using Au and MgO internal pressure standards, *Geophy. Res. Lett.* **33**, L01310 (2003).
43. Sata, N., K. Hirose, G. Shen, Y. Nakajima, Y. Ohishi, and N. Hirao, Compression of FeSi, Fe_3C, $Fe_{0.95}O$, and FeS under the core pressures and implication for light element in the Earth's core, *J. Geophys. Res.* **115**, B09204 (2010).
44. Tange, Y., Y. Nishihara, and T. Tsuchiya, Unified analysis for P-V-T equation of state of MgO: A solution for pressure-scale problems in high P-T experiments, *J. Geophys. Res.* **114**, B03208 (2009).
45. Fei, Y., A. Ricolleau, M. Frank, K. Mibe, G. Shen, and V. Prakapenka, Toward an internally consistent pressure scale, *Proc. Nat. Acad. Sci.* **104**, 9182-9186 (2007).
46. Duffy, T. S., Strength of materials under static loading in the diamond anvil cell, in *Shock Compression of Condensed Matter - 2007* (eds. M. D. Furnish, Elert, M. L., Russell, T. P. and White, C. T.), submitted (AIP, New York).
47. Mao, H. K., J. Xu, and P. M. Bell, Calibration of the ruby pressure gauge to 800 kbar under quasihydrostatic conditions, *J. Geophys. Res.* **91**, 4673-4676 (1986).
48. Chhabildas, L. C., M. D. Furnish, and W. D. Reinhart, Shock induced melting in aluminum: Wave profile measurements, in *Shock Compression of Condensed Matter - 1999* (eds. M. D. Furnish, Chhabildas, L. C. and Hixson, R. S.), 97-100 (AIP, Melville, NY, 2000).
49. Reinhart, W. D., C. LC, and T. J. Vogler, Investigating phase transitions and strength in single-crystal sapphire using shock-reshock loading lechniques, *Int. J. Impact Eng.* **33**, 655-669 (2006).
50. Meade, C. and R. Jeanloz, Yield strenght of Al_2O_3 at high-pressure, *Phys. Rev. B* **42**, 2532-2535 (1990).
51. Chellappa, R., D. M. Dattelbaum, N. Velisavljevic, and S. Sheffield, The phase diagram of ammonium nitrate, *J. Chem. Phys.* **137**, 064504 (2012).

52. Shen, G., Q. Mei, V. B. Prakapenka, P. Lazor, S. V. Sinogeikin, Y. Meng, and C. Park, Effect of helium on structure and compression behavior of SiO_2 glass, *Proc. Nat. Acad. Sci.* **108**, 6004-6007 (2011).
53. Cahill, C. and R. O. Pohl, Thermal conductivity of amorphous solids above the plateau, *Phys. Rev. B* **35**, 4067 (1987).
54. Shenogin, S., A. Bodapati, P. Keblinski, and A. J. H. McGaughey, Predicting the thermal conductivity of inorganic and polymeric glasses: The role of anharmonicity, *J. Appl. Phys.* **105**, 034906 (2009).
55. Hsieh, W. P., M. D. Losego, P. V. Braun, S. Shenogin, P. Keblinski, and D. Cahill, Testing the minimum thermal conductivity model for amorphous polymers using high pressures, *Phys. Rev. B* **83**, 174205 (2011).
56. Chen, B., W. P. Hsieh, D. G. Cahill, D. R. Trinkle, and J. Li, Thermal conductivity of compressed H_2O to 22 GPa: A test of the Leibfried-Sclömann equation, *Phys. Rev. B* **83**, 132301 (2011).
57. Shukla, P., T. Watanabe, J. Nino, J. Tulenko, and S. R. Phillpot, Thermal transport properties of MgO and $Nd_2Zr_2O_7$ pyrochlore by molecular dynamics simulation, *J. Nucl. Mater.* **380**, 1-7 (2008).
58. de Koker, N., Thermal conductivity of MgO periclase from equilibrium first principles molecular dynamics, *Phys. Rev. Lett.* **103**, 125902 (2009).
59. Beck, P., A. F. Goncharov, V. V. Struzhkin, B. Militzer, H. K. Mao, and R. J. Hemley, Measurement of thermal diffusivity at high pressure using a transient heating technique, *Appl. Phys. Lett.* **91**, 181914 (2007).
60. Katsura, T., Thermal diffusivity of periclase at high temperatures and high pressures, *Phys. Earth Planet. Inter.* **101**, 73-77 (1997).
61. Manthilake, G. M., N. de Koker, D. J. Frost, and C. A. McCammon, Lattice thermal conductivity of lower mantle minerals and heat flux from Earth's core, *Proc. Nat. Acad. Sci.* **108**, 17901-17904 (2011).
62. Zha, C. S., H. K. Mao, and R. J. Hemley, Elasticity of MgO and a primary pressure scale to 55 GPa, *Proc. Nat. Acad. Sci.* **97**, 13494-13499 (2000).
63. Stoner, R. J., Kapitza conductance and heat flow between solids at temperatures from 50 to 300 K, *Phys. Rev. B* **48**, 16373-16387 (1993).
64. Lyeo, H. K. and D. G. Cahill, Thermal conductance of interfaces between highly dissimilar materials, *Phys. Rev. B* **73**, 144301 (2006).
65. Hsieh, W. P. and D. G. Cahill, Ta and Au(Pd) alloy metal film transducers for time-domain thermoreflectance at high pressures, *J. Appl. Phys.* **109**, 113502 (2011).
66. Ruckert, T., W. Keune, W. Sturhahn, M. Hu, J. P. Sutter, T. S. Toellner, and E. E. Alp, Phonon density of states in epitaxial FE/CR(001) superlattices, *Hyperfine Interact.* **126**, 363-366 (2000).
67. Mao, Z., J. F. Lin, J. Liu, A. Alatas, L. Gao, J. Zhao, and H. K. Mao, Sound velocities of Fe and Fe-Si alloy in the Earth's core, *Proc. Nat. Acad. Sci.*, in press.
68. Goncharov, A. F., M. Wong, D. A. Dalton, J. G. O. Ojwang, V. V. Struzhkin, Z. Konôpková, and P. Lazor, Thermal conductivity of argon at high pressures and high temperatures, *J. Appl. Phys.* **111**, 112609 (2012).
69. Bennett, K., R. B. Von Dreele, and H.-R. Wenk, 'HIPPO' a new high intensity neutron diffractometer for bulk analysis of materials, *Int. U. Crystallogr. Newsletter* **22**, 6-8 (1999).
70. Kaercher, P., S. Speziale, L. Miyagi, W. Kanitpanyacharoen, and H. R. Wenk, Crystallographic preferred orientation in wustite (FeO) through the cubic-to-rhombohedral phase transition, *Phys. Chem. Minerals* **39**, 613-626 (2012).
71. Doughtery, L. M., E. K. Cerreta, E. A. Pfeif, C. P. Trujillo, and G. T. Gray III, The impact of peak shock stress on the microstructure and shear behaviors of 1018 steel, *Acta Mater.* **55**, 6356-6364 (2007).
72. March, R. A., S. Vukson, S. Surampudi, B. V. Ratnakumar, M. C. Smart, M. Manzo, and P. J. Dalton, Li ion batteries for aerospace applications, *J. Power Sources* **97**, 25-27 (2001).
73. Smart, M. C., B. V. Ratnakumar, K. B. Chin, and L. D. Whitcanack, Lithium-ion electrolytes containing ester cosolvents for improved low temperature performance batteries and energy storage, *J. Electro. Soc.* **157**, A1361-A1374 (2010).
74. Dodd, J. L., I. Halevy, and B. Fultz, Valence fluctuations of ^{57}Fe in disordered $Li_{0.6}FePO_4$, *J. Phys. Chem. C* **111**, 1563-1566 (2007).
75. LeCaer, G. and J. M. Dubois, Evaluation of hyperfine parameter distributions from overlapped Mossbauer spectra of amorphous alloys, *J. Phys. E: Sci. Instrum.* **12**, 1083 (1979).
76. Amthauer, G. and G. R. Rossman, Mixed valence of iron in minerals with cation clusters, *Phys. Chem. Min.* **11**, 37-51 (1984).
77. Achim, C., E. L. Bominaar, J. Meyer, J. Peterson, and E. Munck, Observation and interpretation of temperature-dependent valence delocalization in the $[2Fe\text{-}2S]^+$ cluster of a ferrodioxin from Clostridium pasteurianum, *J. Am. Chem. Soc.* **121**, 3704 (1999).

78. Achim, C., E. L. Bominaar, R. J. Stapes, E. Munch, and R. H. Holm, Influence of extrinsic factors on electron transfers in a mixed-valence Fe^{2+}/Fe_{3+} complex: Experimental results and theoretical considerations, *Inorg. Chem.* **40**, 4389 (2001).
79. Papathanassiou, A. N., I. Sakellis, and J. Grammatikakis, Migration volume for polaron dielectic relaxation in disordered material, *Appl. Phys. Lett.* **91**, 202103 (2007).
80. Goddat, A., J. Peyronneau, and J. P. Poirier, Dependence on pressure of conduction by hopping of small polarons in minerals of the Earth's lower mantle, *Phys. Chem. Min.* **27**, 81-87 (1999).
81. Xu, Y., T. J. Shankland, and A. G. Duba, Pressure effect on electrical conductivity of mantle olivine, *Phys. Earth Planet. Inter.* **118**, 149-161 (2000).
82. Shankland, T. J., J. Peyronneau, and A. T. D. Poian, Electrical conductivity of the Earth's lower mantle, *Nature* **366**, 453-455 (1993).
83. Wu, G. and J. J. Neumeier, Small polaron transport and pressure dependence of the electrical resistivity of $La_{2-x}Sr_xNiO_4$(O<~x<~1.2), *Phys. Rev. B* **67**, 125116 (2003).
84. Holstein, T., Studies of polaron motion: Part II. The "small" polaron, *Ann. Physics* **8**, 343-389 (1959).
85. Lipp, M. J., A. P. Sorini, J. Bradley, B. Maddox, K. T. Moore, H. Cynn, T. P. Devereaux, Y. Xiao, P. Chow, and W. J. Evans, X-ray emission spectroscopy of cerium across the γ-α volume collapse transition, *Phys. Rev. Lett.* **109**, 195705 (2012).
86. Yoo, C. S., A. Sengupta, and M. Kim, Carbon dioxide carbonates in the Earth's mantle: Implications to the deep carbon cycle, *Angew. Chem. Int. Ed.* **50**, 11219-11222 (2012).
87. Gavriliuk, A. G., I. A. Trojan, and V. V. Struzhkin, Insulator-metal transition in highly compressed NiO, *Phys. Rev. Lett.* **109**, 086402 (2012).
88. Baldini, M., V. V. Struzhkin, A. F. Goncharov, P. Postorino, and W. L. Mao, Persistence of Jahn Teller distortion in high pressure metallic phase of $LaMnO_3$, *Phys. Rev. Lett.* **106**, 066402 (2011).
89. Rose, M. C. and R. E. Cohen, Giant electrocaloric effect around T_c, *Phys. Rev. Lett.* **109**, 18764 (2012).
90. Uhoya, W., G. Tsoi, Y. Vohra, N. Wolanyk, S. M. Rao, M. K. Wu, and S. T. Weir, Simultaneous measurement of pressure evolution of crystal structure and superconductivity in $FeSe_{0.92}$ using designer diamonds, *Europhys. Lett.* **99**, 26002 (2012).
91. Sefat, A. S., Pressure effects on two superconducting iron-based families, *Rep. Prog. Phys.* **74**, 124502 (2011).
92. Paglione, J., High-temperature superconductivity in iron-based materials, *Nature Phys.* **6**, 645-658 (2010).
93. Yildirim, T., Strong coupling of the Fe-spin state and the As-As hybridization in iron-pnictide superconductors from first-principle calculations, *Phys. Rev. Lett.* **102**, 037003 (2009).
94. Gretarsson, H., et al., Revealing the dual nature of magnetism in iron pnictides and iron chalcogenides using x-ray emission spectroscopy, *Phys. Rev. B* **84**, 100509(R) (2011).
95. Conner, R. W. and D. Dlott, Ultrafast emision spectroscopy of exploding nanoaluminum in Teflon: Observations of aluminum fluoride, *Chem. Phys. Lett.* **512**, 211-216 (2011).
96. Conner, R. W. and D. Dlott, Comparing boron and aluminum nanoparticle combustion in Teflon using ultrafast emission spectroscopy, *J. Phys. Chem. C* **116**, 2751-2760 (2012).
97. Conner, R. W. and D. D. Dlott, Time-resolved spectroscopy of initiation and ignition of flash-heated nanoparticle energetic materials, *J. Phys. Chem. C* **116**, 14737-14747 (2012).
98. Katsura, T. and E. Ito, Melting and subsolidus phase relations in the MgSiO3-$MgCO_3$ system at high pressures: implications to evolution of the Earth's atmosphere, *Earth Planet. Sci. Lett.* **99**, 110-117 (1990).
99. Isshiki, M., T. Irifune, K. Hirose, S. Ono, Y. Ohishi, T. Watanuki, E. Nishibori, M. Takata, and M. Sakata, Stability of magnesite and its high-pressure form in the lowermost mantle, *Nature* **421**, 60-63 (2004).
100. Dorogokupets, P. I., Equation of state of magnesite for the conditions of the Earth's lower mantle, *Geochem. Int.* **45-46**, 561-568 (2007).
101. Panero, W. R. and J. Kabbes, Mantle-wide sequestration of carbon in silicates and the structure of magnesite II, *Geophy. Res. Lett.* **35**, L14307 (2008).
102. Schrauder, M. and O. Navon, Solid carbon dioxide in a natural diamond, *Nature* **365**, 42-44 (1993).
103. Daschbach, J. L., T. M. Chang, R. Corrales, L. X. Dang, and P. McGrail, Molecular mechanisms of hydrogen-loaded β-hydroquinone clathrate, *J. Phys. Chem. B* **110**, 17291-17295 (2006).
104. Howie, R. T., C. L. Guillaume, T. Scheler, A. F. Goncharov, and E. Gregoryanz, Mixed molecular and atomic phase of dense hydrogen, *Phys. Rev. Lett.* **108**, 125501 (2012).
105. Chen, P. N., C. S. Zha, X. J. Chen, J. Shu, R. J. Hemley, and H. K. Mao, Raman study of phase transitions in compressed methane using moissanite anvil cells, *Phys. Rev. B* **84**, 104110 (2011).
106. Wei, H. and C. S. Yoo, Dynamic responses of reactive metallic structures under thermal and mechanical ignitions, *J. Mater. Res.*, in press.
107. Wei, H., C. S. Yoo, J. Y. Chen, and G. Shen, Oxygen-diffusion limited metal combustions in Zr, Ti and Fe foils: Time- and angle-resolved x-ray diffraction studies, *J. Appl. Phys.* **111**, 063528 (2012).

108. Yoo, C. S., H. Wei, J. Y. Chen, G. Shen, P. Chow, and Y. Xiao, Time- and angle-resolved x-ray diffraction to probe structural and chemical evolution during Al-Ni intermetallic reactions, *Rev. Sci. Instrum.* **82**, 113901-113906 (2011).
109. Jaramillo, R., Y. Feng, and T. F. Rosenbaum, Four-probe electrical measurements with a liquid pressure medium in a diamond anvil cell, *Rev. Sci. Instrum.* **83**, 103902 (2012).
110. Kiefer, B. and T. S. Duffy, Finite element simulations of the laser-heated diamond anvil cell, *J. Appl. Phys.* **97**, 114902 (2005).
111. Kavner, A. and W. R. Panero, Measurement and evaluation of thermoelastic properties in the synchrotron-based laser-heated diamond cell, *Phys. Earth Planet. Inter.* **143-144**, 527-539 (2004).
112. Campbell, A. J., C. T. Seagle, D. L. Heinz, G. Y. Shen, and V. B. Prakapenka, Partial melting in the iron-sulfur system at high pressure: A synchrotron x-ray diffraction study, *Phys. Earth Planet. Inter.* (2007).