CARNEGIE/DOE ALLIANCE CENTER

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

Annual Report
2013-2014

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On the Cover

Clockwise, from top left: 1) Carnegie visiting student Eugene Vinitsky prepares a sample of BaReH$_9$ for investigations of high-pressure phase transitions using Raman and infrared spectroscopy. Vinitsky is spending a year at Carnegie following his undergraduate work at Caltech. 2) Emissivity map across a melted sample of SiC at 12 GPa. Studies of the melting of highly refractory materials is part of the dissertation research of Kierstin Daviau, a graduate student in the group of Academic Partner Kanani Lee at Yale University. 3) Carnegie postdoctoral fellow Caitlin Murphy participates in the 2014 USA Science and Engineering Festival, held in Washington DC. Murphy presented a demonstration on the effects of pressure on materials with defects and impurities. 4) Nearly-pure crystals of acetaminophen are used as models for molecular constituents of plastic-bonded explosives in a collaboration between graduate student John Lazarz and Academic Partner Steve Jacobsen at Northwestern and Dan Hooks, Kyle Ramos and Cindy Bolme at Los Alamos. The collaboration focuses on the use of GHz interferometry to determine high-accuracy elastic constants. 5) Graduate student Emma Rainey, from the group of Academic Partner Abby Kavner at UCLA, presents her work on temperature calibration in the laser-heated diamond anvil cell at the 2013 Fall Meeting of the American Geophysical Union in San Francisco, CA. 6) X-ray diffuse scattering from an Fe-Ga alloy obtained by CDAC Research Scientist Muhtar Ahart at Beamline 16-BM-D at HPCAT confirm the existence of structural inhomogeneity caused by the presence of nanoscale atomic clusters in the solid. Highly optimized diffraction and spectroscopy instrumentation at HPCAT makes possible the investigation of condensed matter at extreme conditions in unprecedented detail.
Carnegie/DOE Alliance Center (CDAC):
A CENTER OF EXCELLENCE FOR HIGH PRESSURE
SCIENCE AND TECHNOLOGY

2013-2014 ANNUAL REPORT

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1. OVERVIEW

Since 2003, the Carnegie-DOE Alliance Center (CDAC) has pushed the frontiers of materials science at extreme conditions through advanced research and training. Headquartered at the Carnegie Institution of Washington (Fig. 1), CDAC is the Center of Excellence for materials within the Stockpile Stewardship Academic Programs of the Department of Energy/National Nuclear Security Administration (DOE/NNSA). The Center continues Carnegie’s tradition of more than a century of advancing fundamental science “for the improvement of mankind,” and in service to the nation, while at the same time promoting unfettered freedom in basic research.1

1.1 CDAC in Year 11

CDAC continues to pursue the core mission articulated at its inception, expanding our understanding of materials behavior at extreme pressure-temperature (P-T) conditions, developing new facilities and methods to advance high P-T materials science, and supporting the education and training of the next generation of scientists in the field. A network of Academic Partners, NNSA Laboratory Partners and Carnegie personnel and facilities comprise the Center. CDAC’s program of education, research and technical development support the fundamental science that underlies the mission of the NNSA in stockpile stewardship and its legacy in national security.2 CDAC personnel study structural, electronic and optical phenomena at extreme conditions in a broad range of materials, including metals, alloys, dense oxides, molecular systems and polymers, and energetic materials - in bulk, on surfaces and at interfaces.

CDAC is managed at Carnegie by Russell J. Hemley (Director), Stephen Gramsch (Coordinator) and Morgan Phillips Hoople (Administrator). CDAC facilities at Carnegie are supported by Research Scientists Maddury Somayazulu, Muhtar Ahart, and Chang-sheng Zha, who support students, postdocs, and visitors from across the Center, including its ofsite facilities (Fig. 2).

At the heart of the CDAC program is the Academic Partner group, 14 faculty representing some of the leading extreme conditions research programs from around the

Figure 1. The Carnegie Institution of Washington’s Broad Branch Road campus celebrated its 100th anniversary this year.

Figure 2. Top to bottom: Advanced Photon Source (APS), the site of the x-ray sector HPCAT; National Synchrotron Light Source (NSLS), the location of IR beamline U2A; and National Synchrotron Light Source II (NSLS II), the site of FIS, the new IR beamline.
CDAC Academic Partners provide the key education and training function of the Center, and prepare highly qualified graduate students for work in areas of fundamental scientific importance for the NNSA mission. CDAC enhances this preparation by providing access to beam time at CDAC-supported facilities, supporting travel to national user facilities for collaboration with other Center participants, and creating opportunities for interaction with students from other groups and with staff from the NNSA Laboratories.

The CDAC partner group has also evolved significantly. We have expanded our program to include more theory and computation in modern high P-T materials science and have added a computational chemist to the Partner group. In addition, at Carnegie, theorist Ivan Naumov has been added as a CDAC Research Scientist. Also, the disciplines pursued by CDAC Partners have become more diverse as the nature of extreme conditions science has expanded in recent years to address an ever-broadening array of problems. Both of these developments promise to enhance the interactions between CDAC groups and scientists in the NNSA Laboratories.

We continue to engage with our Laboratory Partner scientists in high P-T research groups at all three NNSA Laboratories. Our Laboratory Partners serve on the CDAC Steering Committee, providing valuable input on the direction of the scientific program and serve as points of contact in the NNSA Laboratories for our academic groups. The Laboratory Partners also benefit from the availability of discretionary beam time at CDAC user facilities for both programmatic and individual research. They participate in CDAC outreach events and interact directly with graduate students and Academic Partners, providing important insight into the mission and research environment at the NNSA Laboratories.

Researchers throughout the Center can access specialized facilities at HPCAT, the dedicated extreme conditions beamline at the Advanced Photon Source (APS), Argonne National Laboratory (ANL) managed by Guoyin Shen, and U2A, the synchrotron infrared beamline at the National Synchrotron Light Source (NSLS), Brookhaven National Laboratory (Fig. 2) managed by Zhenxian Liu. We are now preparing for the transition to NSLS II and a new IR...
Participants in CDAC also performed experiments at the Lujan Neutron Scattering Center, Los Alamos National Laboratory (LANL). CDAC has supported these DOE/Office of Science (SC) facilities since the inception of the Center in 2003, a fact that highlights one of our important goals—to facilitate partnerships between SC and DOE/NNSA programs. New facilities such as the Dynamic Compression Sector at APS (DCS@APS) and those in the planning stages (MaRIE at LANL), which, along with access to time for fundamental science experiments at Z at Sandia National Laboratories (SNL) and the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory (LLNL), are bringing new capabilities to the field and advancing our understanding of extreme conditions phenomena into new regimes of pressure and temperature.

The overall structure of the Center has proved scientifically productive as well as very effective in achieving our goals in the area of education and outreach (Box 2). On the other hand, the true strength of CDAC has been the results of our efforts at growing the high pressure research community in this country and merging various aspects of it to meet NNSA needs in areas of science crucial to stockpile stewardship.

This report describes the progress of the Carnegie-DOE Alliance Center during the period March 2013-May 2014, including efforts in the Academic Partner groups and among Laboratory Partners. Research of the Laboratory Partners pursued outside CDAC-supported facilities is not addressed.

### 1.2 Highlights from 2013-2014

#### Training, Outreach, and Personnel

- In 2013-2014, CDAC supported the work of 18 graduate students in 14 Academic Partner groups. During this time, 16 CDAC-supported students received the PhD degree, bringing to 41 the total number of degrees earned by CDAC graduate students over the 11 years since the beginning of the Center’s program in 2003.

- At the annual SSAP Symposia in Albuquerque, NM (2013) and Bethesda, MD (2014), CDAC graduate students presented a total of 16 and 17 posters, respectively. In 2013, Best Poster citations were awarded to CDAC students Lisa Mauger (Caltech), Pamela Kaercher (UC-Berkeley), Zeyu Li (Michigan) and Eloisa Zepeda-Alarcon (UC-Berkeley). In 2014, Pamela Kaercher, facility. Participants in CDAC also have performed experiments at the Lujan Neutron Scattering Center, Los Alamos National Laboratory (LANL). CDAC has supported these DOE/Office of Science (SC) facilities since the inception of the Center in 2003, a fact that highlights one of our important goals—to facilitate partnerships between SC and DOE/NNSA programs. New facilities such as the Dynamic Compression Sector at APS (DCS@APS) and those in the planning stages (MaRIE at LANL), which, along with access to time for fundamental science experiments at Z at Sandia National Laboratories (SNL) and the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory (LLNL), are bringing new capabilities to the field and advancing our understanding of extreme conditions phenomena into new regimes of pressure and temperature.

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Emma Rainey (UCLA) and Dane Tomasino (Washington State) received Best Poster Awards (Fig. 4).

- During 2014, CDAC supported the participation of three undergraduate students in Carnegie's Summer Scholars Program, which is supervised by CDAC Coordinator Stephen Gramsch.

- CDAC supported the Paris-Edinburgh Cell Workshop, which was held in May 2013 at APS and hosted by HPCAT. More than 45 participants attended the two-day workshop. The workshop was composed of four technical training courses, and was attended by 32 graduate students, postdocs, and both early career and senior researchers. The unique opportunity provided by the new instrumental setup established at HPCAT was also introduced to the hands-on participants. The workshop was organized by Carnegie's Changyong Park, Yoshio Kono, and Guoyin Shen (HPCAT), along with Yanbin Wang from GSECARS.

- Carnegie Postdoctoral Fellow Caitlin Murphy represented the Geophysical Laboratory at the third annual USA Science and Engineering Festival (Fig. 5). The festival, held April 26-27, 2014 in Washington DC, is the largest science, technology, engineering, and math education event of its kind in the US. Caitlin's topic was "How does high pressure affect materials that have defects and impurities?" Robert Hanrahan, former Program Manager for CDAC at NNSA, discussed stockpile stewardship and non-proliferation at the State Department's booth in the National Security section of the festival.

- CDAC Partners Przemek Dera (University of Hawai'i) and Lowell Miyagi (University of Utah) have been named as the speakers for the 2014-2015 COMPRES Distinguished Lecture series in the field of Mineral Physics. The talks feature topics that emphasize the exciting high-pressure geoscience research being conducted within the COMPRES community and its significance for understanding fundamental Earth and planetary processes. Since its inception in 2008, seven CDAC Academic Partners and/or faculty who were supported as postdoctoral fellows through CDAC have served as Distinguished Lecturers.
CDAC Academic Partner Steven Jacobsen from Northwestern University received a Friedrich Wilhelm Bessel Research Award for 2014. The Bessel Award is granted by the Alexander von Humboldt Foundation, and allows the recipient to spend a year working at a research institution in Germany. He will spend the coming year at the Bayerisches Geoinstitut in Bayreuth, Germany, where he was a Humboldt Postdoctoral Fellow from 2002-2004.

Eva Zurek, a CDAC Academic Partner from the University at Buffalo received the 2014 Young Leaders Professional Development Award of The Minerals, Metals and Materials Society (TMS). She was presented with the award at the 2014 annual meeting of the TMS in San Diego, CA.

Scientific Program

A group including CDAC Partner Hans-Rudolf Wenk, current CDAC students Pamela Kaercher and Eloisa Zepeda-Alarcon, and former CDAC student Jane Kanitpanyacharoen from UC-Berkeley carried out high P-T diffraction experiments on polycrystals to explore in situ crystallographic orientation development and changes during the α→ω and ω→α phase transitions in Zr. Viscoplastic Self-Consistent modeling of uniaxial compression data shows that upon decompression, the ω-phase reverts back to the α-phase with a texture identical to that of the starting phase, documenting a perfect texture memory after cycling through the ω phase.  

CDAC graduate student Kierstin Daviau from Yale has carried out a multi-technique, high P-T investigation of the highly refractory material SiC using new experimental capabilities, including a 4-color temperature mapping technique in the laboratory of CDAC Academic Partner Kanani Lee (Fig 6). Preliminary results show that at low pressures and below 1500 K, SiC forms a new phase, and then decomposes to Si and C at higher temperatures.

A group from Lawrence Livermore National Laboratory and UC-Berkeley, including current and former CDAC Academic Partners Raymond Jeanloz and Tom Duffy, former Carnegie-CDAC Postdoc Amy Lazicki (LLNL) and CDAC Steering Committee members Jon Eggert and G. W. (Rip) Collins (both from LLNL), carried out ramp compression experiments on carbon to 5 TPa at the National Ignition Facility. In these experiments, data was obtained on carbon at peak stresses of 2.7, 3.7 and 5 TPa, resulting in a 3.7-fold compression of the material and a density of 12 g/cm³, greater than the density of lead at ambient pressure.

In recent work at Carnegie, CDAC Director Russell Hemley, and Research Scientist Chang-sheng Zha, together with Carnegie’s Ronald Cohen, report Raman measurements on hydrogen and deuterium to 325...
GPa at 300 K, which provide structural information on hydrogen with increasing density along the I-III-IV transition pathway. Changes in intensities and linewidths of the hydrogen vibron with increasing pressure are accompanied by discontinuities in pressure shifts, which indicate changes in structure and bonding, molecular orientation and electronic structure in the compressed solid. The results further point to the formation of new phases, which may be either completely new structures, or variations of the structure of phase IV.\textsuperscript{6}

- Experiments carried out by Yue Meng (HPCAT) and co-workers from Carnegie and colleagues from George Mason University, Oak Ridge National Laboratory, and Tohoku University successfully identified a liquid-liquid phase transition in Ce metal. At 13 GPa, upon increasing temperatures from 1550 to 1900 K, a high-density liquid transforms to a low-density liquid, with a density change of 14%. Theoretical results suggest that the transition is first order and terminates in a critical point. Computational work further points to the delocalization of $f$ electrons and a fluctuation in the valence state of the Ce atom as the origin of the transition to a low-density liquid state at high pressure and temperature.\textsuperscript{7}

- CDAC graduate student Jinhyuk Lim from the Schilling group at Washington University in St. Louis carried out four-point electrical resistivity measurements on Dy metal up to 157 GPa and has observed a record-high magnetic ordering temperature between 400–500 K at this pressure. The ordering temperature increases dramatically at $P > 73$ GPa, at which pressure the volume decreases by 6%. The highest previously observed ordering temperature was 292 K at ambient pressure for gadolinium metal (Fig. 7).\textsuperscript{8}

- CDAC graduate student Spencer Smith, along with CDAC Partner Yogesh Vohra and colleagues from the University of Alabama – Birmingham used Raman spectroscopy, synchrotron x-ray diffraction (XRD), and \textit{ab initio} harmonic frequency calculations to explore the solid-state transition behavior of paracetamol (Fig. 8) a commonly used analgesic and anti-pyretic) at hydrostatic pressures up to 21 GPa. The results of this work are being used by the pharmaceutical industry to understand pressure-induced phase transitions that take place at low pressure during the tableting process.\textsuperscript{9}

- Muhtar Ahart (Carnegie) and CDAC Director Russell J. Hemley, along with colleagues from Virginia Tech and the National Institute for Standards and Technology, employed high-pressure XRD techniques to investigate the phase behavior of Fe$_{0.81}$Ga$_{0.19}$ alloy (Galfenol) (Fig. 9) at 300 K. Diffuse scattering measurements carried out at...
beamline 16-BM-D at HPCAT reveal that a coarsening-resistant, nanometer-scale clustering of bulk defects is responsible for enhanced magnetostriective behavior in the alloy as compared to pure iron. The work explains earlier suggestions of an underlying structural in homogeneity proposed on the basis of earlier neutron diffraction results.\textsuperscript{10}

- Long-standing discrepancies in the melting curves of refractory metals have been addressed at Carnegie with the use of an advanced laser flash-heating technique. Predoctoral fellow Amol Karandikar and Carnegie’s Reinhard Boehler concurrently developed an analysis procedure that has reduced the uncertainty in the melting curve of Ta metal to less than 200 K.

- UCLA graduate student Emma Rainey has quantitatively explored the temperature gradients in laser-heated diamond anvil cells using numerical modeling techniques. Rainey’s model solves the steady-state heat conduction equation over the sample chamber, gasket, and diamond anvils. The results show that laser heating in a "flat-top" mode does not produce a temperature gradient that is flatter or more uniform than would be produced by a Gaussian beam profile of similar width.\textsuperscript{11}

- CDAC Partner Steve Jacobsen (Northwestern), CDAC Research Scientist Zhenxian Liu (NSLS) and colleagues from the University of New Mexico, University of Southern California, and University of Wyoming used a unique combination of synchrotron IR spectroscopy, TEM, numerical modeling, and seismic P\textsuperscript{-}to\textsuperscript{-}S conversions recorded by a dense seismic array in North America to examine the effects of downwelling from the transition zone into the lower mantle. In experiments, the transition of hydrous ringwoodite to perovskite and (Mg,Fe)O produces intergranular melt. Detections of abrupt decreases in seismic velocity where downwelling mantle is inferred are consistent with partial melt below 660 kilometers. These results suggest hydration of a large region of the transition zone and that dehydration melting may act to trap H\textsubscript{2}O in the transition zone.\textsuperscript{12}

**Technique Development**

- The Frontier Synchrotron Infrared Spectroscopy (FIS) Beamline under Extreme Conditions has been approved as one of the eight NxtGen beamlines to be developed and constructed at NSLS-II (Fig. 2). FIS is the successor of the IR facility (U2A) at NSLS, the highly productive, Carnegie-managed user facility supported by COMPRES and CDAC, and the only dedicated high-pressure synchrotron IR facility in the world. Construction of the beamline hutch on bending magnet port 22 will be completed and all existing equipment at U2A moved in by early 2015.

- The laser shock compression facility operated by the Diott group at Illinois has undergone several improvements. The group has added a femtosecond IR laser which can now be used to carry out IR absorption spectroscopy of shocked solids and liquids. Also under development is a 1 ns, 32 channel optical pyrometer that can be used to study the temperature dynamics of shocked materials.

- Graduate student Lisa Mauger, from the Fultz group at Caltech, has developed a specialized furnace that can be interfaced to beamline 16-ID-D at HPCAT to carry out NRIXS measurements at elevated temperature. The work was carried
Figure 11. A) Single-crystal hydrous ringwoodite (blue crystal) containing 1 wt% H₂O inside a DAC at 30 GPa. The sample was laser-heated to 1600°C in several spots (orange circles) to perform direct transformation to perovskite and (Mg,Fe)O. B) Spectrum 1 is an unheated spot, characteristic of hydro ringwoodite. Spectra 2 and 3 show characteristics of OH in quenched glass. C) On conversion to perovskite plus (Mg,Fe)O, dehydration melting occurred as inter granular melt.

out in collaboration with former CDAC student Matt Lucas at the Air Force Research Laboratory.

- A recently installed quad-diode beam position monitor and feedback software on beamline 16-ID-D at HPCAT ensures a stable beam position, and optimizes the intensity of the beam on the sample, both critical in high pressure spectroscopy experiments.

- On beamline 16-BM-B at HPCAT, Nenad Velisavljevic (LANL) has led the development of simultaneous XRD, x-ray radiography, electrical resistance, and thermal measurements with the Paris-Edinburg (PE) cell along with student Jason Baker and beamline staff at HPCAT. Preliminary experiments have shown that the apparatus performs with high efficiency up to 6 GPa and 1000°C.

- At HPCAT beamline 16-ID-B, progress continues on the development of techniques for time-resolved diffraction. Rapid on-line data analysis has been achieved through optimizing existing software to generate high-quality pressure-temperature-volume relations. An area detector prototype with imaging capability of 800 Hz has been tested and allows the collection of data for compression rates exceeding tens of TPa/s (Fig. 10).

- A group led by Wenge Yang (HPSynC) and including researchers from Carnegie, the APS, and University College London has used a new signal averaging technique to eliminate the severe distortions of the high-energy x-rays employed in x-ray imaging to study a 400 nm gold nanocrystal to 6.4 GPa. The averaging algorithm, used on data from APS beamline 34-ID-C, improves spatial resolution over previous methods by more than two orders of magnitude.  

2. SCIENTIFIC PROGRESS

1. High P-T Phase Relations and Structures
2. P-V-T EOS Measurements
3. Phonons, Vibrational Thermodynamics and Elasticity
4. Plasticity, Yield Strength and Deformation
5. Electronic and Magnetic Structure and Dynamics
6. High P-T Chemistry

2.1 High P-T Phase Relations and Structures

Dehydration Melting in the Deep Earth — The high water storage capacity of minerals in Earth’s mantle transition zone (410- to 660-kilometer depth) implies the possibility of a deep H₂O reservoir, which could cause dehydration melting of vertically flowing mantle. Ongoing work in the group of CDAC Partner Steve Jacobsen (Northwestern) seeks to model these processes using high P-T techniques. Together with Carnegie-CDAC Research Scientist Zhenxian Liu (NSLS) and colleagues from the University of New Mexico, University of Southern California, and University of Wyoming, the group has used a unique combination of synchrotron infrared spectroscopy, TEM,
numerical modeling, and seismic P-to-S conversions recorded by a dense seismic array in North America to examine the effects of downwelling from the transition zone into the lower mantle. In experiments, the transition of hydrous ringwoodite to perovskite and (Mg,Fe)O produces intergranular melt (Fig. 11). Detections of abrupt decreases in seismic velocity where downwelling mantle is inferred are consistent with partial melt below 660 kilometers. These results suggest hydration of a large region of the transition zone and that dehydration melting may act to trap H₂O in the transition zone.¹²

**Phase Transitions in Relaxor**

**Ferroelectrics** – Relaxor ferroelectrics such as Pb(Mg₀.₃NB₂₀₉)O₃–x–PbTiO₃ (PMN-PT) solid solutions show not only superior piezoelectric properties but also broad frequency dispersive dielectric properties with a low concentration of PT. On the other hand, the PbZr₁₋ₓTiₓO₃ system behaves similarly to normal ferroelectrics such as PbTiO₃. Many of these materials exhibit structural transitions under pressure.¹⁴ For example, PbTiO₃ undergoes second order phase transitions at 12 GPa at 300 K and 16 GPa at 10 K.¹⁵ Carnegie’s Muhtar Ahart has shown that the structural transitions in the PbZr₁₋ₓTiₓO₃ system at 9 GPa are driven by soft mode behavior.¹⁶ Diffraction data were combined with the results of Raman scattering measurements to uncover the transition mechanism.

Diffraction measurements were carried out at HPCAT beamlines 16-ID-B and 16-BM-D. Raman scattering, which was carried out at Carnegie, allowed observation of optical phonons near the Γ point of the Brillouin zone, revealing dynamics that occur in nm sized local structure. Analysis of the spectra was carried out according to the well-established procedure of Lima *et al.*¹⁷ Assignments for the monoclinic phase at ambient pressure are shown in Fig. 12.

These results suggest that the transition from the monoclinic to the rhombohedral phase in PbZr₀.₅₄Ti₀.₄₆O₃ at 3 GPa is related to octahedral tilting, but the second transition that takes place at 9 GPa is driven by a soft optical phonon. The higher pressure transition around 27 GPa, which involves a drastic change in the Raman spectrum and a splitting of diffraction peaks, is associated with a lower symmetry transition. It is proposed that the third transition is from a centro-symmetric rhombohedral to a possible monoclinic or orthorhombic phase induced by pressures above 27 GPa.

**High-Pressure Melting of SiC** – CDAC graduate student Kierstin Daviau at Yale is carrying out a multi-technique study of the high-pressure, high-temperature behavior of silicon carbide (SiC) melting using new techniques developed in the laboratory of Academic Partner Kanani Lee.¹⁸ SiC melting at high pressures is not well understood, and existing

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Figure 12. Detailed display of Raman spectra of PbZr₁₋ₓTiₓO₃ at selected pressures. Dashed lines are guides to the eye.

Figure 13. Cross section of β-SiC quenched from 30 GPa and heated to temperatures of ~2600 K. Note darker crystals, measured by EDS to be C-rich. Scale bar is 2 μm.
studies have inconsistent findings, particularly concerning the Clapeyron slope for the melting curve. Given the discrepant results, it has not been clear whether SiC melts congruently (i.e., SiC solid \(\rightarrow\) SiC liquid) or incongruently (e.g., SiC solid \(\rightarrow\) Si liquid + C solid). It appears that at low temperatures (less than \(\sim\)1500 K), SiC sluggishly forms a new solid phase, still undetermined, that has been observed via Raman spectroscopy and XRD. Additionally, it appears that upon further heating, SiC breaks down. Diffraction shows evidence of lonsdaleite, a high pressure polymorph of carbon, and scanning electron microscopy, shows small grains of carbon intermixed within a SiC matrix (Fig. 13). While it appears that it has been possible to melt SiC, investigation of the additional phases and the possible dissociation of SiC at high pressures and temperatures is ongoing.

Experiments with the laser-heated diamond anvil cell (DAC) are challenging, but practical with DAC technology. Due to the small sample chamber size (~10s to 100s of microns) and the high thermal conductivity of diamond, large radial and axial temperature gradients have long plagued DAC experiments. This is due to the thinning of thermal insulation layers that surround the sample against the effects of the highly conductive diamonds at high pressure. In order to overcome these constraints, short-duration laser heating, along with an updated four-color temperature mapping measurement technique (Fig. 6) have been developed, and electron microscopy of quenched samples is used to observe texture and composition. In order to investigate heating along the compression direction, focused ion beam milling techniques allow viewing a cross section of each sample, making features due to melting easier to identify.

**New Findings in Dense Hydrogen** — Using the U2A facility at NSLS, Chang-sheng Zha, Zhenxian Liu, Muhtar Ahart, Reinhard Boehler, and Russell Hemley have examined the structure, bonding and electronic properties of highly compressed hydrogen. Experimental results (Fig. 14) show that one type of molecule interacts very weakly with its neighboring molecules, which is unusual for molecules at this very high compression. The other type of molecule bonds with its neighbors, forming surprising planar sheets that comprise the structure. The measurements also show that solid hydrogen at these conditions is on the borderline between a semiconductor and a semimetal. The results disprove earlier claims that hydrogen forms a dense atomic metal at 300 GPa and room temperature.\(^\text{19}\)

As a result of recent advances in DAC techniques, measurements on hydrogen to above 300 GPa at room temperature are now possible. Raman measurements of hydrogen and deuterium to 325

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**Figure 14.** Left: Selected synchrotron IR spectra at different temperatures in the vicinity of the vibrons. (a) Isobaric measurements of 268 GPa through the III-IV phase transition. (b) Detail in the vibron region at 280 GPa and 295 K. (c) Isothermal compression showing the evolution of the spectrum through phases III and IV at 300 K. The fitted lines show the peaks attributed to each phase. The bar gives the absorbance scale for each panel. Right: Phase diagram of hydrogen to multimegabar pressures.
GPa at 300 K, representing new regimes of pressure and temperature, have been carried out by Zha and Hemley, together with Carnegie’s Ronald E. Cohen and Ho-kwang Mao. These measurements provide structural information on hydrogen with increasing density along the I-III-IV transition pathway. A detailed analysis of the spectra indicate that transitions in hydrogen proceed by the formation of a sequence of disordered stackings of molecular and distorted layers. Changes in intensities and linewidths of the hydrogen vibron with increasing pressure (Fig. 15) are accompanied by discontinuities in pressure shifts, which indicate changes in structure and bonding, molecular orientation and electronic structure in the compressed solid. The results further point to the formation of new phases, which may be either completely new structures, or variations of the structure of phase IV. Further work will seek to not only clarify known regions of the phase diagram and explore new pressure-temperature regimes, but also to improve existing theoretical models.

**Boron Carbide under Pressure** – Because of its outstanding hardness, thermodynamic stability, low density, and electronic properties, boron carbide has many uses: i.e. as a refractory material, in abrasive powders and ballistics, as a neutron radiation absorbent, and in electronic applications. The space group of boron carbide is generally suggested to be $R3m$, and it is thought to be composed of icosahedra and three atom chains. However, the broad range of compositions possible (from 8-20 at. % carbon) coupled with the fact that it is impossible to distinguish between boron and carbon using diffraction, leaves many open questions about the structure of boron carbide at 1 atm. In addition very little is known about its behavior under hydrostatic pressure. CDAC graduate student Andrew Shamp at Buffalo has worked towards predicting the most stable structures and important metastable species of boron carbide in a wide pressure range (1 atm – 10 TPa), and studied their electronic structures. The work carried out to date has focused on the idealized carbon-rich $B_4C$ stoichiometry. In the most stable structure found in DFT calculations, the linear chain has a ‘CBC’ arrangement, and one carbon atom is found in the polar site (Fig. 16). Interestingly, this phase becomes unstable with respect to decomposition into pure carbon and boron around 50

**Figure 15.** Hydrogen vibron spectra across the I-III-IV transition.\(^{19}\)

**Figure 16.** Top right: the CBC\(_p\) configuration shown is the most stable structure below 50 GPa. At higher pressures, segregated boron and carbon are enthalpically preferred. Top left: the same CBC\(_p\) configuration with a Wannier function describing one of the carbon sp\(^3\) hybrid orbitals in the chain. This Wannier function shows the bond between the chain carbon and polar boron in the icosahedron. Bottom left: CDAC graduate student Andrew Shamp (Buffalo).
GPa, but it remains dynamically stable up to at least 100 GPa. Shamp and CDAC Partner Eva Zurek are currently analyzing the response of different structures to pressure. In most configurations the three atom chain is predicted to bend, and linearity is only maintained in a structure containing a CCC motif. The configuration which is the most stable at 1 atm remains enthalpically preferred under pressure. This structure also shows the greatest bending of the CBC chain, and it therefore has the smallest volume. Using qualitative analysis techniques (such as generation of 'Fat bands', COHPs and Wannier functions via the LMTO and NMTO methods), it is possible to get a better understanding of the electronic structure of various phases under pressure.

**Structure and Physical Properties of Hydrogen-Bearing Post-Perovskite** – CDAC graduate student Joshua Townsend (Northwestern) is carrying out experiments and theoretical calculations on hydrogen incorporation into the post-perovskite structure of MgSiO$_3$, which may be stable at the core-mantle boundary. By studying the effects of chemical substitutions on post-perovskite material properties at extreme conditions, results are being applied to interpreting the heterogeneous seismic structure of the core-mantle boundary region. Using density functional theory, Townsend has found a stable hydrogen defect structure of post-perovskite containing 1600 ppm H$_2$O. Vibrational and elastic properties have been calculated for the structure up to 120 GPa, showing an 8% reduction in the bulk modulus for the H-bearing structure compared with ideal MgSiO$_3$ (Fig. 17). At the NSLS beamline U2A, in collaboration with Zhenxian Liu, Townsend has co-developed a new CO$_2$ laser heating system, which he is using to try and synthesize hydrogen-bearing post-perovskite for comparison with his theoretical calculations. Through chemical interactions at the core-mantle boundary, primordial hydrogen from the core may enter the post-perovskite structure and influence properties of the core-mantle boundary including viscosity, electrical conductivity, and melting.

**Liquid-Liquid Critical Point in Ce Metal** – Understanding polymorphism in liquids provides key insights into the complex nature of the liquid state, and may now be studied in detail as a result of advances in synchrotron XRD techniques. The observation of a liquid-liquid transition in a material having two distinct liquid phases of differing density is experimentally challenging and requires simultaneous high pressure and high temperature conditions and instantaneous capture of the diffuse scattering from both liquid phases. Recent experiments carried out by Yue Meng (HPCAT), and co-workers from Carnegie, along with colleagues from George Mason University, Oak Ridge National Laboratory, and Tohoku University have now successfully identified a liquid-liquid phase transition in cerium metal.

At 13 GPa, upon increasing temperatures from 1550 to 1900 K, a high-density liquid transforms to a low-density liquid (Fig. 18) with a density change of 14%. Theoretical results suggest that the transition is first order and terminates in a critical point (LLCP). Computational work
further points to the delocalization of $f$ electrons and a fluctuation in the valence state of the Ce atom as the origin of the transition to a low-density liquid state at high pressure and temperature.\(^7\)

**Giant Magnetostriction in Fe-Ga Alloy** –
Galfenol is a new class of iron-based, magnetic Fe\(_{1-x}\)Ga\(_x\) alloy that exhibits giant magnetostriction and has attracted considerable attention because of its potential for use in mechanical devices where resistance to fracture is an important criterion. Maximum values of the magnetostriction coefficient (3/2\(\lambda\)) of 400 ppm (more than one order of magnitude higher than that for pure \(\alpha\)-Fe) have been observed in bulk single crystals with \(x = 0.19\). A structurally heterogeneous model has been proposed to explain the enhanced magnetostriction and elastic softening for Fe\(_{1-x}\)Ga\(_x\) alloys. This model assumes that heat treatment produces a structurally and chemically heterogeneous state consisting of coarsening-resistant, nanometer-scale DO\(_3\) precipitates in FeGa alloy. Recent neutron diffuse scattering measurements on FeGa alloys confirm that the enhanced magnetostriction is directly related to the presence of an underlying structural heterogeneity.

Motivated by a strong interest in understanding the effects of pressure on these materials, CDAC Research Scientist **Muhtar Ahart** and CDAC Director **Russell J. Hemley**, along with colleagues from Virginia Tech and the National Institute for Standards and Technology, employed high-pressure XRD techniques to investigate the phase behavior of the Fe\(_{0.81}\)Ga\(_{0.19}\) alloy at 300 K. The goal was to study determine how the addition of Ga affects the pressure-induced bcc-to-hcp phase transition in Fe, how pressure affects the diffuse scattering, and to search for new phases in order to uncover the underlying microscopic mechanism responsible for the giant magnetostriction.
in the alloy. XRD measurements were carried out at HPCAT beamline 16-BM-D. The x-ray measurements reveal several interesting facts: (1) The bcc-to-hcp phase transition pressure of 18.5 GPa (Fig. 1) for single-crystal Fe_{0.81}Ga_{0.19} is 6.5 GPa higher than that for pure iron (13 GPa). (2) The pressure of the bcc-to-hcp phase transition on compression and decompression differs by roughly 10 GPa, whereas for pure iron this difference is only 5 to 6 GPa; such hysteretic behavior is characteristic of martensitic transformations. (3) The volume difference between the cubic and hexagonal phases of Fe_{0.81}Ga_{0.19} at the transition point is much smaller than that for pure iron (Fig. 19, left); this itself is very interesting and indicates the strong effect of adding Ga. (4) Remarkably clear diffuse scattering (Fig. 19, right) was observed in the 300 μm thick samples, and this diffuse scattering is associated with the DO_{3} precipitates.

By analogy with the phase transition in pure iron, a mechanism for the transition is proposed in which the hcp structure can be derived from the bcc lattice through a compression along the [001] direction, followed by shear along the [1-10] direction. An explanation consistent with experimental observations is that the larger atomic size of Ga is responsible for the higher bcc-to-hcp transition pressure compared to that for pure iron. A modest uniaxial stress of ~3 GPa is sufficient to suppress the presence of DO_{3} nanoprecipitates, and eliminate diffuse scattering.

2.2 P-V-T EOS Measurements

**Carbon to 50 Megabars** – Increased study of the nature of planetary interiors, as well as the current effort to produce inertial confinement fusion, both call for an understanding of matter at ultra-dense states, characterized by pressures in the TPa range. The possible existence of carbon-rich planets has created interest in the behavior of carbon at these conditions. Pursuing this work is a group from Lawrence Livermore National Laboratory and UC-Berkeley, including current and former CDAC Academic Partners Raymond Jeanloz and Tom Duffy, former Carnegie-CDAC Postdoc Amy Lazicki (LLNL) and CDAC Steering Committee members Jon Eggert and G. W. (Rip) Collins (both from LLNL). Ramp compression experiments on carbon have been carried out to 5 TPa at the NIF. NIF, which houses the world’s largest and most powerful laser, was constructed to realize inertial confinement fusion of hydrogen as an energy source, but discovery science experiments are also provided time on the facility through a proposal review process.

In the experiments at NIF, 176 laser beams converge simultaneously onto a hohlraum target, which converts the ultraviolet radiation to x-rays; the x-rays ablate the sample and result in dynamic compression of the material. Four thicknesses of the diamond sample effectively allow multiple sample runs within the same experiment (Fig. 20). Velocity interferometry is then used to create a stress-density profile that characterizes the load on the sample. Because ramp compression is more controlled than shock compression, NIF allows observations in pressure ranges where shock compression data are unreliable and static compression data are not available. In these experiments, data was obtained on carbon at peak stresses of 2.7, 3.7 and 5 TPa, resulting in a 3.7-fold compression of the material and a density of 12 g/cm^3, greater than the density of lead at ambient pressure. One of the primary uses of the data obtained at NIF is to provide stringent tests of modern condensed matter theory and models of planetary formation. The LLNL team is also collaborating with the CDAC group at Carnegie on experiments on hydrogen and hydrogen-containing compounds to be carried out at NIF in the future.

**Temperature Distribution in the Laser-Heated DAC** – One of the key goals of the Kavner group at UCLA is pressure and temperature calibration of laser-heating experiments using
the DAC, and to elucidate the principles governing the mechanical behavior of engineering materials at ultrahigh pressures and high temperatures. While previous efforts have focused on mechanical properties of composite materials at high pressures in the diamond cell, during the past two years the CDAC-supported effort in the group has shifted focus toward studying the temperature distribution in the laser heated DAC, and the mechanical properties of samples subject to both high pressures and temperatures.

To design experiments and test hypotheses, CDAC graduate student Emma Rainey has created and validated a 3-D numerical model, TempDAC, for calculating temperature distributions within the laser-heated DAC (LHDAC) applicable to continuous wave laser heating experiments. TempDAC solves the steady-state heat conduction equation over the sample chamber, gasket, and diamond anvils. Sample geometries, laser beam profiles, and laser absorption properties are flexible, allowing TempDAC to accurately model a wide range of experimental conditions. Thermal conductivities in TempDAC are both material- and temperature-dependent, and can also be anisotropic.

Example calculations illustrate several interesting properties of the extreme temperature gradients that form during DAC laser heating experiments, and underscore the need for considering heat conduction in three dimensions when predicting LHDAC temperature gradients and interpreting XRD data obtained during laser heating. In particular, the results show that a “flat-top” laser beam, while it can produce a shallow temperature gradient near the center of the sample, does not produce a temperature gradient that is flatter or more uniform than would be produced by a Gaussian beam profile of similar width (Fig. 21).

![Figure 21. Left, calculated radial temperature profiles at the surface of a Pt foil for flat-top (black line and symbols) and Gaussian (blue line and symbols) laser beams. Right, corresponding axial temperature profiles through the center of the sample. Inset: CDAC graduate student Emma Rainey (UCLA).](image)

**Paracetamol’s Hidden Polymorphs** – The study of the behavior of polymorphic organic solids at high pressure is a relatively new and rapidly growing area of interest. The applications span a wide ranging field which includes the pharmaceutical industry, where often times different crystal phases of the same drug can have different physiological effects.

CDAC Graduate Student Spencer Smith, along with CDAC Academic Partner Yogesh Vohra and colleagues from the University of Alabama - Birmingham, used Raman spectroscopy, synchrotron XRD, and multiple ab initio harmonic frequency calculations to explore the solid-state
transition behavior of paracetamol (a commonly used analgesic and anti-pyretic) at hydrostatic pressures up to 21 GPa (Fig. 8).

Spectral measurements provide further evidence for a highly kinetically driven Form I — Form II transition occurring as a mixed phase from 4.8 to 6.5 GPa, as well as new evidence for previously unobserved Form IV and Form V occurring at pressures of 8.1 and 11 GPa, respectively.  

Unexpected Densities of Bulk Metallic Glasses – In any material, the increase in density with decreasing volume is directly related to the nature of the interatomic interactions. For typical crystalline materials, the volume varies as the cube of the change in interatomic distance. In amorphous materials, however, an irregular network of interatomic interactions can lead to deviations from this well-established relationship. For bulk metallic glasses (BMGs), a 2.3 (as opposed to the expected 3) power law relationship has been proposed based on studies of materials with different compositions. At high pressure, however, the problem of accurate measurement of density and volume in the DAC has made such studies difficult (Fig. 22).

In recent work at HPCAT 16-BM-D, a group from Carnegie and Stanford has used a unique combination of XRD, ultrasonic interferometry/x-ray radiography and transmission x-ray microscopy to determine the density and volume of BMGs at high pressure. Studies of several different compositions from 0.7 up to 22 GPa show that a 5/2 power law relationship describes the compression behavior of BMGs quite closely, suggesting a universal type of behavior for these and perhaps other, related materials.

2.3 Phonons, Vibrational Thermodynamics, and Elasticity

Pressure Dependence of the Thermal Conductance of Interfaces between Highly Dissimilar Materials – CDAC student Greg Hohensee from the Cahill group at Illinois is combining the experimental techniques of time-domain thermoreflectance (TDTR) and the high-pressure environment of DACs to advance fundamental understanding of the thermal conductivity of materials and the thermal conductance of interfaces. TDTR is an optical pump-probe technique that can be used to measure the thermal conductivity of almost any type of material with a smooth surface. The high spatial resolution of TDTR enables measurements of samples with volumes as small as 10×10×1 μm³. Cahill’s group has previously shown that weak interfacial bonding can suppress G by an order of magnitude below the value predicted by conventional models. Anvil cell techniques can easily generate pressures (typically 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. As the strength of interface bonding increases at high pressures, G of weakly-bonded interfaces approaches the thermal conductance of clean and strongly-bonded interfaces between materials.
Currently, the focus is on a long-standing problem in the field of nanoscale thermal transport: when the phonon spectra on the two sides of the interface are highly dissimilar, the observed values for $G$ are much larger than the maximum predicted by elastic (harmonic) phonon-scattering\textsuperscript{24, 25} the so-called “phonon-radiation-limit” (PRL). The phonon-radiation-limit is reached when the transmission coefficient of phonons incident on the interface from the material with high vibrational frequencies is close to unity for all phonon frequencies that are below the upper cut-off frequency $\Omega$ of the vibrational spectrum in the material with low vibrational frequencies. The conductance in the phonon-radiation-limit scales with $\Omega^3$. If the thermal conductance greatly exceeds the phonon-radiation-limit, the usual assumption in the field has been that inelastic (anharmonic) interactions between phonons create additional channels for heat transport. In the prototypical example of Pb/diamond, the assumption is that one phonon in diamond interacts with two (or more) phonons in Pb. The radiation limit for this type of three-phonon process is simply $2^3 \times 8$ times larger than the conventional elastic phonon radiation limit. Theoretical understanding of the magnitude of the inelastic channel is lacking.

High pressure provides a method of varying the phonon frequencies and anharmonicity of materials and therefore we can gain new insight on this long-standing problem by measuring how $G$ varies with pressure. Data for interfaces between Pb, Au(Pd), Pt, and Al metal films and diamond at pressures up to 50 GPa are compiled in Fig. 23. The upper cut-off frequency $\Omega$ increases in the sequence Pb, Au, Pt, to Al. (The Au(Pd) film is a dilute alloy of Pd in Au that is used to increase the optical absorption of Au.) Data for Al closely resemble the phonon-radiation limit. The deviation between the data and phonon radiation limit becomes larger as $\Omega$ decreases. For Pb/diamond, the deviation is on the order of a factor of 8 at all pressures.

For some samples, the conductance increases steeply at first, presumably because of stiffening of weak interfacial bonding as we previously observed for Al/graphene/SiC interfaces.\textsuperscript{23} In all cases, the conductance at high pressure is flatter than the trend predicted by the phonon radiation limit. Work is ongoing to understand this weak pressure dependence. The working
hypothesis is that there are competing effects: i) pressure increases $\Omega$ and therefore enhances the elastic channel for heat transport and ii) pressure decreases the anharmonicity of the metal and therefore reduces the inelastic channel for heat transport.

In the case of Au(Pd), an additional contribution to $G$ may be coming from the relatively low lattice thermal conductivity $\Lambda_l$ combined with the small value of the electron-phonon coupling parameter $g$. The series conductance created by electron-phonon non-equilibrium near an interface is given by $G_{\text{NE}}=(g\Lambda_l)^{1/2}$. For Au at ambient pressure, $G_{\text{NE}}\approx 300$ MW m$^{-2}$ K$^{-1}$. $\Lambda_l$ is expected to increase with pressure and to decrease with pressure. Current work focuses on an evaluation of the variation in $G_{\text{NE}}$ with pressure and the importance of $G_{\text{NE}}$ in these measurements.

Interestingly, the thermal conductivity of the Type 1A diamonds, $\approx 500$ W m$^{-1}$ K$^{-1}$, is a factor of 4-5 smaller than the intrinsic value, and $\approx 2000$ W m$^{-1}$ K$^{-1}$ for Type 2A diamonds. Characterization by infrared spectroscopy suggests that the Type 1A anvils contain approximately 1500 ppm of nitrogen impurities. These impurities strongly suppress thermal conductivity and could potentially reduce $G$ because of a greater mismatch between the phonons that carry heat across the interface and the phonons that carry heat in the diamond crystal. That phonon non-equilibrium effect, if present, is not obvious in the data. The conductance of interfaces with diamond appears to be insensitive to the diamond purity.

**Nonharmonic Vibrational Properties of $\alpha$-Fe** – The thermodynamics of iron and its phase transitions are of longstanding interest. The entropy of iron originates with the degrees of freedom of phonons, electrons, and spins, and is also affected by interactions between them. Vibrational entropy makes the largest contribution to the high temperature thermodynamics of metallic iron, and the vibrational entropy can be obtained directly from the phonon density-of-states (DOS) obtained by nuclear resonant inelastic x-ray scattering (NRIXS).

During the last year CDAC student Lisa Mauger at Caltech completed a substantial experimental effort to study the vibrational properties of bcc Fe and their impact on the thermodynamics. This included the development of a new high temperature NRIXS furnace in collaboration with former CDAC student Matthew Lucas (Air Force Research Lab). The furnace was commissioned at AFRL and used for GUP / CDAC beamtime at HPCAT in April 2013 to collect NRIXS spectra of bcc Fe and cementite (Fe$_3$C) at elevated temperatures.

The detailed study of the phonon DOS of iron at 38 temperatures between 30K and the fcc transition at 1184K showed that bcc iron has a significant nonharmonic contribution to the vibrational entropy. It is poorly modeled by the quasi-harmonic theory typical of conventional *ab-initio* calculations. It does not track the typical trends of phonon-phonon anharmonicity, either, and there is little thermal broadening of the spectrum. By elimination, this leaves a large magnon-phonon interaction in bcc iron as anomalous source of phonon entropy. In fact, the anharmonic contribution to the vibrational entropy of bcc Fe tracks the magnetic entropy as shown in Fig. 24. Evidently a large magnon-phonon coupling in bcc iron makes a significant contribution to the

![Figure 24](image_url)
Beyond the thermodynamic analysis, a genetic algorithm optimization to extract interatomic force constants from our phonon DOS measurements has also been implemented. The model optimizes Born-von Karman interatomic force constants through a least-squares comparison with the measured phonon DOS, providing information on interatomic interactions. These force constants were also used to generate phonon dispersions at elevated temperatures that were in excellent agreement with the few triple axis neutron studies of phonons in iron at high temperature.\textsuperscript{26} The thermal trends in our phonon dispersions exhibit anomalously large anharmonic behavior at some points in k-space (e.g., $T_2[\xi\xi\xi]$ in Fig. 25) while other phonons were as expected from quasiharmonic estimates ($L[\xi\xi\xi]$ in Fig. 25). The rapid softening of the second nearest neighbor axial force constants in iron near the magnetic transition corresponds with the observed rapid softening of the low energy transverse $\Gamma$-N phonon branch ($T_2[\xi\xi\xi]$ in Fig. 25). Apparently the magnon-phonon interaction has considerable variation in k-space.

**Elastic and Mechanical Properties of Boron-Doped Diamond** – Among various dopants possible in diamond, boron is important because at modest levels boron-doped diamond is a semiconductor. CDAC graduate student **Yun-Yuan Chang**, along with postdoctoral researcher **Xiaobing Liu**, at Northwestern University, are investigating the influence of boron on diamond’s elastic and mechanical properties. Using GHz-ultrasonic interferometry, the elastic constants of boron-doped diamond with a gradient of boron concentration is currently under investigation. In regions with

![Figure 25. Energies of specific phonon modes versus temperature. The modes are compared with their quasiharmonic estimates (gray dashed lines).](image1)

![Figure 26. Top left: boron-doped diamond with a compositional gradient spanning one order of magnitude, from about 100 to 1000 ppm boron. The crystal measures 2 mm across. Spatially resolved acoustic and mechanical properties measurements are being carried out at Northwestern to correlate the influence of defects on elastic properties of semi-conducting, single-crystal boron-doped diamond. Top right: comparison of the anisotropy of Poisson’s ratio between natural type Ia diamond (red curve) and heavily boron-doped diamond (>2000 ppm), blue curve. The figure was calculated from the elastic tensor measured by GHz-ultrasonic interferometry. The result illustrates how boron reduces the elastic moduli of diamond as well as its elastic anisotropy. Bottom left: CDAC graduate student Yun-Yuan Chang (Northwestern).](image2)
relatively low boron (150-300 ppm) the bulk and shear moduli are 444(3) and 530(2) GPa, respectively. Whereas, in regions of higher boron concentration (Fig. 26, top left) dark blue areas in the figure, 1500-2000 ppm B), the elastic moduli are reduced to about 436(3) GPa (bulk) and 521(2) GPa (shear). Experimental studies of hardness are currently underway, with preliminary results showing that the Vicker’s hardness in high-boron doped region is measurably lower than in the low-boron region (Fig. 26, top right). The research will further the understanding of how defects influence elastic properties of superhard materials and further inform relationships between mechanical and elastic properties.

High P-T Elastic Properties of Majorite Garnet – CDAC graduate student John Lazarz (Northwestern) is using online Brillouin scattering at the APS to measure the sound velocities of majorite garnet at simultaneous high pressure and high temperature conditions of the Earth’s mantle. The majorite, nominally Mg$_3$(Fe,Al,Si)$_2$(SiO$_4$)$_3$, also contains hydrogen at the level of ~1000 ppm, so the experiments are testing the influence of H-related defects on the elastic properties of this important mantle phase. In the transition zone (410-660 km depth), observed seismic velocities appear too fast to be explained by the standard mantle rock model, called dry pyrolite. It is possible that H$_2$O, incorporated into the high-pressure phases of the transition zone could reduce velocities to better match seismic observations. Because majorite is slower than the co-existing ringwoodite (spinel), a higher basaltic (majorite-rich) component in the mantle from descending slabs could also reduce velocities to better match observations. These experiments on the sound wave velocities of majorite at pressures up to 15 GPa and 700 K will thus be useful for placing tighter constraints on the composition of the Earth’s mantle. Lazarz has constructed a resistive-heated DAC for the measurements.

Brillouin Spectroscopy of CaSiO$_3$ – A Brillouin study of CaSiO$_3$ glass carried out by CDAC graduate student Zack Geballe at Berkeley provides evidence that amorphous CaSiO$_3$, though metastable at room temperature, is a thermodynamic phase in the sense that it can be described by a single energy surface, $G(P,T)$, independent of synthesis conditions. The proposed energy surface is consistent with observed transitions between amorphous and crystalline phases at both low and high pressures, and consistent with the acoustic measurements (Fig. 27) that constrain the curvature of energy versus pressure. The acoustic data thus constrain the Gibbs free energy estimates for crystalline and amorphous phases.

Single-Crystal Elastic Constants of Molecular Crystals – Knowledge of elastic constants of molecular crystals is important in the area of energetic materials used in plastic-bonded explosives. In particular, accurate determination of constituent material properties of heterogeneous media will improve mesoscale simulations of growth and formation of hot spots during weak initiation. CDAC Academic Partner Steve Jacobsen and graduate students Yun-Yuan Chang and
heat is conducted in the deep lower mantle, 660 to 2,900 kilometers below the surface. CDAC postdoctoral associate Allen Dalton (now at Defense Threat Reduction Agency), Carnegie’s Alexander Goncharov, CDAC Academic Partner David Cahill (Illinois), and CDAC students Gregory Hohensee and Wen-Pin Hsieh, have for the first time experimentally measured the conductivity of a key Earth material (MgO) at these conditions. The results suggest that heat transfer in Earth’s mantle is lower than other predictions, with total heat flow across the Earth of about 10.4 terawatts, which is about 60% of the power used today by civilization. Conductivity also has less dependence on pressure conditions than predicted.

This work provides important bounds on the degree to which heat is transferred by convection as opposed to conduction in the lower mantle. Further work will focus on examining the effects of different mineral components on the thermal conductivity and to better understand the atomic scale basis of convective motion of these materials within the broader context of mantle dynamics. The results suggest that this technique could advance other high pressure and temperature studies of the deep Earth and provide a better understanding of the finer details of Earth’s evolution.27

2.4 Plasticity, Yield Strength and Deformation

Deformation of Hexagonal Metals at High Pressure – For many years, the Wenk group at Berkeley has been interested in phase transitions in metals, and particularly orientation relations if materials are under stress and at high pressure. The original DAC deformation experiments on iron,28 and more recent work29 were used to understand seismic anisotropy in the Earth’s

**Figure 28.** Single-crystal acetaminophen (bottom right) synthesized by the LANL group for GHz-ultrasonic measurements (0.5-2 GHz) at Northwestern to determine the elastic tensor. Acoustic waveforms from different polarizations taken at 1 GHz are shown. Top right: CDAC graduate student John Lazarz (Northwestern).
inner core. Since then investigations have moved on to deformation mechanisms in other hexagonal metals at high pressure.\textsuperscript{30} Transition metals Ti, Zr, and Hf have a hexagonal close-packed structure (α) at ambient conditions, but undergo phase transformations with temperature and pressure. Of particular significance is the high-pressure ω phase which is brittle compared to the α phase (Fig. 29). There has been a long debate about transformation mechanisms and orientation relations between the two crystal structures, but new high pressure DAC and D-DIA experiments resolved this with \textit{in situ} synchrotron XRD texture studies on polycrystalline aggregates.\textsuperscript{3} Following crystal orientation changes in Zr confirmed that the original suggestion for an α → ω martensitic transition for Ti, with (0001)\textsubscript{α} || (11\bar{2}0)\textsubscript{ω}, and a remarkable orientation memory when ω reverts back to α.

\textbf{Deformation and Transformation Textures in NaMgF\textsubscript{3} Perovskite and Post-Perovskite} – MgSiO\textsubscript{3} post-perovskite (pPv) is believed to be the major phase in the Earth’s lowermost mantle. Thus it is critically important to understand the plastic deformation properties of pPv in order to understand the rheology and seismic anisotropy of this region. However, the MgSiO\textsubscript{3} system is difficult to study due to the extreme pressures needed to stabilize the pPv phase (~130 GPa). Furthermore, current high temperature deformation DAC technology is limited to P-T conditions of ~65 GPa and ~2000 K,\textsuperscript{31} thus deformation behavior of MgSiO\textsubscript{3} pPv currently cannot be studied at high pressure and temperature. Over the last year CDAC graduate student Michael Jugle at Utah has been studying high pressure texture development in NaMgF\textsubscript{3} perovskite (Pv) and pPv as a potential analog system for MgSiO\textsubscript{3} Pv and pPv. Previously, transformation textures in NaMgF\textsubscript{3} during the phase transformation from Pv to pPv have been documented. Texture changes during the phase transformation indicate that \{100\}Pv → \{110\}pPv. This transformation relation is consistent with previous theoretical and experimental work on the Pv to pPv transformation mechanisms.\textsuperscript{32-35} In February 2014, deformation experiments were performed on NaMgF\textsubscript{3} pPv up to 66 GPa at HPCAT. Figures 30a and 30b show the results of the deformation experiment. After transformation at 37 GPa, NaMgF\textsubscript{3} pPv exhibits a transformation texture with a maximum near 110. Upon compression to 66 GPa this texture disperses and develops a maximum toward 001 with a minimum near 100. To determine the deformation mechanisms associated with this texture change, polycrystal plasticity modeling using the Visco-Plastic Self Consistent (VPSC) code was performed. The transformation texture shown in Fig. 30a was used as a starting texture for the simulations. Results for dominant (010)<101> slip and (001)<100> slip are shown in Figs. 30c and 30d.

\textbf{Figure 30.} Top: inverse pole figures of NaMgF\textsubscript{3} pPv from experiment (a, b) and from VPSC simulations (c, d). a, transformation texture immediately after conversion from the Pv phase. b, texture after compression to 66 GPa. c and d, simulations for dominant (010)<101> slip and dominant (001)<100> slip respectively. Dominant (001)<100> provides the closest match to (b). Pole densities are given in multiples of random distribution (m.r.d.) where an m.r.d. of 1 is random and a higher number indicates a greater number of orientations (stronger texture). Left: CDAC graduate student Michael Jugle (Utah).
(010)<101> slip has been previously observed in CaIrO$_3$ pPv and (001)<100> slip has been inferred for MgGeO$_3$ and MgSiO$_3$ pPv. (010)<101> slip generates a strong maximum at 010 and a minimum at 001 as in Fig. 30c. Slip on (001)<100> results in a maxima near 110 with a shoulder close to 001 (Fig. 30a), similar to the experimental deformation texture (Fig. 30b). It is thus concluded that NaMgF$_3$ pPv slips predominantly on the (001) plane. This is consistent with MgSiO$_3$ pPv providing strong evidence that NaMgF$_3$ is a good analog for deformation behavior of MgSiO$_3$ pPv, and a good candidate for future high P-T deformation experiments.

**Deformation of Two Phase Materials**

The Utah group has recently been joined by summer undergraduate intern Max Giannetta, who is working closely with Michael Jugle to analyze diffraction data from deformation experiments on mechanical mixtures with a range of volume fractions of NaCl + MgO. The Earth’s lower mantle is composed of primarily MgSiO$_3$ pPv (~70-80 vol %) and MgO (~30-20 vol %). MgSiO$_3$ pPv is believed to be the mechanically harder phase while MgO is believed to be the softer phase. These experiments on the simple solids NaCl and MgO seek to elucidate the fundamental deformation behavior of polyphase materials with a phase contrast, and to determine which phase controls deformation, in particular how texture development is affected by the presence of a harder or softer phase. Texture analysis has been performed on the first of these compression datasets, a mechanical mixture of 75 vol. % NaCl + 25 vol. % MgO (Fig. 31). In this experiment, NaCl rapidly develops a 100 texture maximum with a shoulder toward 110, consistent with slip on {110}<1-10>. Unsurprisingly MgO, which is the harder phase and volumetrically minor remains essentially random. Thus the majority of strain is partitioned into the softer NaCl and MgO is only passively involved in deformation. At pressures greater than ~30 GPa, the B1 to B2 transformation in NaCl is observed. By 34 GPa, the transformation to B2 is complete. The B2 phase of NaCl exhibits a texture maximum at 110 with a shoulder toward 111. This indicates transformation relationships of {001}B1 → {110}B2 and {110}B1 → {111}B2 consistent with previously proposed mechanisms for B1-B2 transformations based on molecular dynamics simulations.

**Deformation of Polyphase Materials**

Despite recent progress, polyphase deformation is still very enigmatic. In the Wenk group at Berkeley, DAC experiments on periclase + perovskite mixtures and D-DIA experiments on
mantle analogs are ongoing, along with modeling simulations in collaboration with Ricardo Lebensohn and Carlos Tome at LANL. It turns out that in such mixtures preferred orientation development is highly reduced due to local stress-strain heterogeneities. Figure 32 shows results of a fast Fourier transform model that documents that heterogeneous Von Mises strain concentrates on the soft phase, while the hard phase barely deforms. These are important components of the PhD thesis of Pamela Kaercher. Eloisa Zepeda-Alarcon is continuing with the project. A comparative microtomography study on the same samples at APS, ALS and SLS documented amazing resolution and reproducibility. The Wenk group has dedicated considerable effort in making their sophisticated diffraction data analysis more widely available. Tutorials on Rietveld texture analysis have recently been published.

2.5 Electronic and Magnetic Structure and Dynamics

Parallel Suppression of Superconductivity and Fe Moment in Sr-substituted CaFe$_2$As$_2$ – The Fe-pnictide superconductors present systems that challenge the notion of the antithetical nature of superconductivity and magnetism. These systems are composed of corrugated Fe-As layers arranged in a tetragonal unit cell, and at low temperature, they display antiferromagnetic order. With doping or pressure, however, the antiferromagnetism can be suppressed, and superconductivity can develop.

Jason Jeffries from LLNL has been carrying out non-resonant Fe K$_\beta$ x-ray emission spectroscopy (XES) experiments at HPCAT 16 ID-D of the APS, which reveal that Sr substitution into CaFe$_2$As$_2$ decouples the Fe moment from the volume collapse transition, yielding a collapsed-tetragonal, paramagnetic normal state out of which superconductivity develops (Fig. 33). XRD measurements at Sector 16 BM-D implicate the c-axis lattice parameter as the controlling criterion for the Fe moment, promoting a generic description for the appearance of pressure-induced superconductivity in the alkaline-earth-based 122 ferropnictides (AFe$_2$As$_2$). This work suggests that both the destruction of antiferromagnetism and the presence of the Fe moment are requisite for the development of high-temperature superconductivity in these systems. That the pressure-dependent suppression of $T_c$ tracks that of the Fe moment supports the picture of an unconventional superconducting state mediated by magnetic fluctuations. This generic picture suggests that driving the CT phase to ambient pressure while maintaining an Fe moment should be a promising route to high-temperature, magnetically mediated superconductivity in the 122 systems.

High Pressure Effects on the Superconductivity in Rare Earth Doped CaFe$_2$As$_2$ – High pressure superconductivity in a rare-earth doped Ca$_{0.86}$Pr$_{0.14}$Fe$_2$As$_2$ single crystal sample has been studied up to 12 GPa and temperatures down to 11 K using designer DAC technology under quasi-hydrostatic pressure conditions. The electrical resistance measurements were complemented by high pressure and low temperature XRD studies at HPCAT 16 BM-B. Electrical resistance measurements show an intriguing observation of superconductivity under pressure, with $T_c$ as high as $\sim$51 K at 1.9 GPa, presenting the highest $T_c$ reported in the intermetallic class of 1-2-2 iron-based superconductors (Fig. 34). The resistive transition observed suggests the possible existence of two superconducting phases at 0.5 GPa: one phase starting at $T_{c1} \sim$ 48 K and
Figure 34. Left: Temperature dependence of the electrical resistance of rare earth doped Ca$_{0.86}$Pr$_{0.14}$Fe$_2$As$_2$ at various applied pressures. Steatite was used as the pressure medium. The two superconducting transitions ($T_{c1}$ and $T_{c2}$) are clearly observed at low pressures below 2 GPa. Right: Variation of measured superconducting transition temperatures $T_{c1}$ and $T_{c2}$ for Ca$_{0.86}$Pr$_{0.14}$Fe$_2$As$_2$ with pressure.

**Robust Ferromagnetism in the Compressed Permanent Magnet Sm$_2$Co$_{17}$** – Permanent magnets have found applications since antiquity, but the purview of their technological impact has exploded in recent decades. Most of this newfound application space has been enabled by the development, and subsequent deployment, of high-strength permanent magnets based on intermetallic compounds composed of rare-earth (RE) and transition-metal (TM) elements. The compound Sm$_2$Co$_{17}$ displays magnetic properties amenable to permanent magnet applications owing to both the 3$d$-electrons of Co and the 4$f$-electrons of Sm. The long-standing description of the magnetic interactions between the Sm and Co ions implies a truly ferromagnetic configuration, but some recent calculations challenge this, suggesting at least a propensity for ferrimagnetic behavior. **Jason Jeffries** from LLNL has used high-pressure synchrotron x-ray techniques to characterize the magnetic and structural properties of Sm$_2$Co$_{17}$. The results reveal a robust ferromagnetic state. Ly XES at Sector 16 ID-D has been used to probe the Sm $f$-state under pressure. The local Sm moment is at most weakly affected by compression. These results, combined with data from x-ray magnetic circular dichroism (XMCD) and XRD experiments, indicate that the ordered moments show a surprising resilience to volumetric compressions of nearly 20%.

**Magnetic Properties of Rare Earth Materials at High Pressures** – During the past year, CDAC graduate student **Jinhyuk Lim**, from the Schilling group at Washington University in St. Louis, has made progress in the understanding of magnetism in rare earth materials through several different projects.

**Record High Magnetic Ordering Temperature in Dy at 157 GPa:** In some of the most precise four-point measurements of the electrical resistivity ever obtained at extreme pressure (see Fig. 7), **Lim** has succeeded in subjecting the lanthanide metal Dy to pressures as high as 157 GPa. After initially decreasing under pressure and passing through a minimum near 20 GPa, Dy's magnetic ordering temperature $T_o$ begins to increase dramatically for $P > 73$ GPa, the pressure at which Dy's volume suddenly collapses by 6%. As the pressure increases further, $T_o$ increases through ambient temperature near 110 GPa, reaching at 157 GPa an estimated maximum value of 400 - 500 K, by far the highest ordering temperature of any lanthanide, the highest previous value being $T_o = 292$ K for Gd at ambient pressure.

The reason for this dramatic increase appears to be that Dy under extreme pressure enters a Kondo lattice or dense Kondo state. The negative mixing exchange interaction associated with this state becomes anomalously large as Dy is pushed by pressure toward a magnetic instability, leading to the record high value of the magnetic ordering temperature.
In contrast, the lanthanide metal Gd shows no such anomalous pressure dependence of $T_o$ for pressures just above 59 GPa where its volume collapses. The extreme magnetic stability of Gd does not allow the Kondo lattice to develop so that the magnetic ordering temperature follows a conventional pressure dependence where, under extreme pressure, $T_o$ never comes close to reaching its ambient pressure value of 292 K. These experiments were carried out in collaboration with Gilberto Fabbris and Daniel Haskel at the APS.

**Pressure-Induced Volume Collapse in Gd and Tb:** Most elemental lanthanide metals suffer a volume collapse at a critical pressure, for Gd at 59 GPa and for Tb at 53 GPa. There is much controversy regarding the mechanism(s) responsible for this volume collapse. Candidates are: (a) valence change, (b) 4f local-itinerant transition, (c) Kondo resonance, (d) s-d electron transfer. X-ray absorption near-edge structure (XANES) and XES measurements at the APS by G. Fabbris et al.\textsuperscript{8} on Gd and by Maddox et al.\textsuperscript{43} on Tb speak against (a) and (b). The true state of the lanthanide ion under pressure can be inferred from the degree of suppression of the superconductivity in a very dilute magnetic alloy for pressures just exceeding the critical pressure for the volume collapse. Experiments by Gilberto Fabbris and Jinhyuk Lim on the dilute magnetic alloys Y(0.5 at.% Tb) and Y(0.5 at.% Gd) reveal that there is very strong suppression of superconductivity only in the former alloy. One can infer that the volume collapse in Tb can be best described by the Kondo volume collapse model of Allen and Martin,\textsuperscript{44} whereas in Gd the volume collapse arises from simple $s$-$d$ charge transfer \cite{5} under pressure. Very recent parallel experiments on Dy and the dilute magnetic alloy Y(1 at.% Dy) lead to the same conclusions as for Tb.\textsuperscript{45}

**Pressure-Quenched Dense Kondo State in CeB\textsubscript{6}:** CeB\textsubscript{6} is a well-known dense Kondo system, as evidenced by its temperature-dependent electrical resistivity that initially decreases on cooling from ambient temperature and passes through a "Kondo" minimum near 100 K before rising steeply to a sharp maximum near 6 K and then dropping precipitously (see Fig. 35 at 0.5 GPa). However, the application of 43 GPa pressure changes this behavior (Fig 35). The highly anomalous temperature dependence of the resistivity is completely suppressed, leaving only conventional Fermi-liquid-like behavior to the highest pressure studied (122 GPa).\textsuperscript{46}

The primary reason for studying this compound under extreme pressure was to search for a transition to possible topological insulating behavior as has been observed for SmB\textsubscript{6} at ambient pressure. Although this transition was not observed in the present experiment, the destruction of the dense Kondo state is also of considerable interest since its evolution can be continuously tuned using pressure as a parameter. These measurements...
Synthesis of Nanophase Diamond with NV Centers – Nanodiamond (ND) synthesis has a variety of applications such as biological markers, drug delivery facilitation, and nanotesla metrology.\(^4^7\) Metrology and biological markers use the coherent properties and optical polarization of the negatively charged Nitrogen Vacancy center defect (NV\(^-\)). At Carnegie, visiting graduate student Todd Zapata from Texas A & M has been working on the synthesis of nanodiamond with NV\(^-\) centers using adamantane, C\(_{10}\)H\(_{16}\), and its nitroxyl radical (2-azaadamantane-N-oxyl), which are shown in the inset of Fig. 36. Ultimately, the material may be used as an in-situ sensor for measuring very weak magnetic signals from DAC samples. The synthesis is carried out using the DAC and either laser or resistive heating. The ultimate goal of this work is to work out the growth conditions that will produce the smallest possible ND which may at the same time hold NV\(^-\) centers (~ 5 nm), with as little agglomeration as possible, and coherence which rivals the NV\(^-\) center in bulk diamond. Raman spectroscopy is used to follow the evolution of the adamantane-nanodiamond transition. \(T_1\) and \(T_2\) coherence times of the NV\(^-\) centers are measured using Hahn Echo experiments. Anti-bunching experiments are performed to determine the number of NV\(^-\) centers per ND, and AFM/SEM images are taken to determine the size and agglomeration of the ND. The analysis of the NV\(^-\) is carried out at the University of Ulm with the help of Fedor Jelezko.

Although this project is still in its early stages, there have been several important results thus far. With regards to synthesis, it is necessary to include hydrogen within the DAC sample chamber to terminate the ND and hinder the transformation of ND to onion-like carbon. Raman analysis (532 nm excitation) confirms the existence of nanometer-sized diamonds from the shift in the diamond peak to about 1326 cm\(^{-1}\). There is typically also a large shoulder following the diamond peak centered around 3120 cm\(^{-1}\) (Fig. 36) due to fluorescence from the NV\(^-\). Some of the ND also exhibits a strong Raman peak in the 1420 cm\(^{-1}\) range, which is associated with the neutral NV (NV\(^0\)).
2.6 High P-T Chemistry

Hydrides with Novel Stoichiometries – It is widely believed that metallic hydrogen will be superconducting at high temperatures. One way to metallize hydrogen may be to access the appropriate region of the temperature/pressure phase diagram. However, a chemical route towards this ‘holy grail’ is also being sought out. One may wonder if compressed hydrogen can be metallized via doping by a particular element, if the resulting phases also have the propensity to be superconducting at high temperatures, and if they could be stabilized at 1 atm. In order to advance research in this field Andrew Champ at Buffalo has computationally studied mixtures of hydrogen and iodine under pressure. At 150 GPa, the H$_2$I and H$_2$I stoichiometries become thermodynamically stable. In the H$_2$I phase the iodine atoms form buckled triangular nets. Bonding between the nets results in a host structure, and 1-D chains of H$_2$ molecules with slightly stretched bonds (0.80 Å) behave as the guests. H$_2$I consists of layers of H$_2$ molecules (which measure 0.81 Å) arranged in a hexagonal lattice, with the I atoms forming layers below and above the hexagons. It resembles the AlB$_2$ structure, where iodine assumes the position of the aluminum atoms, and the center of the H$_2$ bond is found in the same spot as boron.

Calculations reveal that at 150 GPa H$_2$I has a high DOS at $E_F$ hinting that it may be superconducting.

Calculations of the $T_c$ of H$_2$I are currently underway

Furthermore, Andrew has worked with other members of the Zurek group to predict the structures of the strontium polyhydrides, SrH$_n$ with $n>2$, under pressure. A number of phases with even $n$ were found to be thermodynamically stable below 150 GPa. Particularly interesting is the SrH$_4$ stoichiometry (Fig. 38), which comprises the convex hull at 50, 100, 150 GPa. Its hydrogenic sublattice contains H$_2$ and H units, and throughout the pressure range considered it adopted one of the two configurations which were previously predicted by for CaH$_4$ under pressure. At 150 GPa, the SrH$_6$ stoichiometry has the lowest enthalpy of formation. The most stable configuration assumes $P3$ symmetry, and its lattice consists of one-dimensional H$_2$···H hydrogenic chains. Symmetrization of these chains results in the formation of [H] helices, which are reminiscent of the trigonal phase of sulfur. The $R3m$-SrH$_6$ phase, which is comprised of these helices, becomes dynamically stable by 250 GPa, and has a high density of states at the Fermi level.

We explored the geometric relationships between $R3m$-SrH$_6$ and the $Im3m$-CaH$_6$ and $Imm2$-BaH$_6$ structures found in prior investigations. High Pressure Kinetic Studies using the Dynamic DAC – Current research supported by CDAC in the group of Academic Partner Choong-shik Yoo at Washington State focuses on the study of solid-state transformations and dense solid-solid interfaces of multi-phases and/or mixtures, across the melting/solidification, phase transitions, amorphization, and chemical reactions, utilizing the dynamic-DAC (d-DAC) coupled with time-resolved spectroscopy and time-resolved synchrotron XRD. The d-DAC is capable of precise controls of pressure and compression rates in time-scales that are ideal for diffusion-controlled solid-state transformations, complementing conventional DAC and shock wave studies. To probe the structural evolution of solids undergoing phase and chemical
changes, the d-DAC is coupled with time-resolved Raman spectroscopy, time-resolved synchrotron XRD, and time-resolved high-speed microphotography. Combining with a pulse (or ramp) laser-heating method, it is possible to produce tailored dynamic thermo-mechanical conditions for specific transformations of interest such as dynamic shear-induced deformation, interfacial mixing and bonding, and structural and chemical transformations. This work has been the focus of the dissertation research of CDAC graduate student Dane Tomasino.

**Melting and Phase Transitions in Ramp-Heated Nitrogen at High Pressures** – Raman studies of nitrogen were performed to investigate the melting curve and solid-solid phase transitions in the pressure-temperature range of 25 to 103 GPa and 300 to 2000 K. The solid-liquid phase boundary has been probed with time-resolved Raman spectroscopy on ramp-heated nitrogen in the DAC, showing a melting maximum at 73 GPa and 1690 K. The solid-solid phase boundaries have been measured with spatially resolved micro-confocal Raman spectroscopy in the resistively heated DAC, in order to investigate the δ-ε phase line to 47 GPa and 914 K. At higher pressures the θ-phase was produced upon a repeated thermal heating of the ζ-phase, yet no evidence was found for the υ-phase.

**Time-Resolved XRD across Phase Transitions in H₂O** – The d-DAC with time-resolved XRD (Fig. 39) to determine time evolutions of structural and chemical changes in H₂O under rapidly modulating pressures across a series of phase transitions (HDW—metastable ice VII—HDA—ice VI—ice VII, HDW = high density water, HAD = high density amorphous ice) over a wide range of compression rates (10² to 10⁴ GPa/s). We have obtained a large number of time-resolved x-ray data on H₂O, and the major findings include: The structural evolution of ice VI to ice-VII, however, occurs rather coarsely. The diffraction data shows an anisotropic compression behavior of ice VI; the c-axis is more compressible than the a-axis at the same compression rate. Nevertheless, the present equations of state of both ice VI and ice VII obtained under dynamic loadings agree well with those previously obtained under static conditions.⁵⁰

**Characterization of a Mineral-Fluid Interface by X-ray Reflectivity** – Termination and hydration of the forsteritic (Fo₉₀Fa₁₀) olivine (010) surface have been investigated by Changyong Park at HPCAT with high-resolution specular x-ray reflectivity and atomic force microscopy under room temperature and pressure conditions. The surface was prepared by polishing a naturally grown (010) face, which was found in an acidic (pH 3.5) alumina suspension to exhibit regular steps while the basic (pH 9.5) silica polished surface is irregularly roughened. This indicates that there are two distinguishable mechanochemical processes for the surface dissolution. The quantitative interpretation of the regular steps from the alumina-polished surface suggests that the observed step heights correspond to multiples of the crystallographic unit cell. The terrace surface was investigated with high-resolution specular x-ray reflectivity to determine the termination and hydration conditions (Fig. 40). The model-dependent fit of the reflectivity data suggests that the alumina-polished olivine (010) surface in equilibrium with water is terminated at a partially depleted (~24% with respect to stoichiometric) M1 metal atom plane. Vacancies created by this depletion and the removal of surface SiO₄ oxygen atoms are filled by adsorbed water species. The terminating plane
Figure 39. Dye emission redshift transients at different pressures (impact velocities) with (a) 25 μm thick flyers, (b) 50 μm thick flyers (c) 75 μm thick flyers and (d) 100 μm thick flyers. The dashed line at 7 ns in (a) is a guide to the rising edge. The dashed lines at 10 ns in (b)-(d) indicate the change in slope associated with the transition from elastic to viscous compression.

Figure 40. A) Model of interface structure. B) Electron density profile from fit.

The structural phase stability of N-(4-hydroxyphenyl) acetamide (paracetamol, Fig. 8) has been studied by CDAC graduate student Spencer Smith (UAB) at ambient temperature up to 12 GPa using Raman spectroscopy. Spectral changes have provided further evidence for a highly kinetically driven Form I → II transition that occurs as a mixed phase from 4.8 – 6.5 GPa, and might be completed as low as 7 GPa. Upon further compression to 8.1 GPa, a drastic shift in spectral signature was observed providing the first evidence for a previously undiscovered Form IV of paracetamol. Additional shifts in nanomaterials (e.g., Al + Fe2O3) by detecting and time-resolving the burst of light that accompanies initiation.\(^5\) Also under investigation are the complex material dynamics of a high molecular weight polymer using noninvasive emissive spectroscopic probes embedded in the polymer.\(^5\) As shown in Fig. 41, the dye emission spectrum is monitored, while an algorithm assists in the computation of the emission peak redshift versus time. The figure shows how the peak shift varies with time in PMMA for different shock pressures and different flyer speeds. This work is part of the dissertation research of CDAC graduate students Will Shaw and Will Bassett (Fig. 42).

**Shock Initiation of Reactive Nanomaterials**

During the past year, the Dlott group at Illinois has been using their laser-launched flyer plate apparatus (see section 4) to study shock initiation of reactive nanomaterials (e.g., Al + Fe2O3) by detecting and time-resolving the burst of light that accompanies initiation.\(^5\) Also under investigation are the complex material dynamics of a high molecular weight polymer using noninvasive emissive spectroscopic probes embedded in the polymer.\(^5\) As shown in Fig. 41, the dye emission spectrum is monitored, while an algorithm assists in the computation of the emission peak redshift versus time. The figure shows how the peak shift varies with time in PMMA for different shock pressures and different flyer speeds. This work is part of the dissertation research of CDAC graduate students Will Shaw and Will Bassett (Fig. 42).
mode intensities were observed near 11 GPa indicating a potential restructuring of the hydrogen bonding network and/or structural modification to a potentially new Form V. Multiple\textit{ab initio} harmonic frequency calculations at different levels of theory were performed with a B3LYP/6-31G** basis set used to provide a more robust mode assignment to experimentally obtained Raman modes. High pressure XRD was performed up to 21 GPa which provided further evidence for a highly kinetically driven Form I $\rightarrow$ II transition in agreement with Raman measurements. In addition, the XRD provided further evidence for the existence of Form IV near 8 GPa and Form V near 11 GPa with Form V persisting up to 21 GPa.

### 3. EDUCATION, TRAINING, AND OUTREACH

CDAC works to support the education and training of the next generation of scientists for work in areas of fundamental science that are important for Stockpile Stewardship. In addition to direct support of graduate students in the Academic Partner groups, we also seek opportunities to support outreach to the broader high pressure community in the US.

#### 3.1 CDAC Graduate Students and Postdoctoral Fellows

The primary focus of CDAC is the support of graduate student preparation in the groups of the Academic Partners. As outlined in our technical section, CDAC graduate students pursue many different types of problems in areas of high $P$-$T$ research relevant to stockpile stewardship, and their work represents the fields of materials science, physics and chemistry as well as high-pressure mineral physics and geophysics. One-third of the CDAC award goes to the support of graduate students in our Academic Partner groups. To date, 41 students have received the PhD degree with either full or partial support from CDAC.

During 2013-2014, the following graduate students were supported either fully or in part through CDAC for their work toward the PhD degree in the groups of in the research groups of CDAC Academic Partners.

- **Caltech (Fultz)**
  - Lisa Mauger
  - Max Murialdo

- **UC-Berkeley (Wenk)**
  - Eloisa Zepeda-Alarcon
  - Pamela Kaercher

- **Alabama–Birmingham (Vohra)**
  - Spencer Smith
  - Samuel Moore

- **Illinois (Dlott)**
  - Will Shaw
  - Will Bassett

- **Yale (Lee)**
  - Kierstin Daviau

- **UCLA (Kavner)**
  - Emma Rainey

- **Northwestern (Jacobsen)**
  - Yun-yuan Chang
  - John Lazarz

\textbf{Figure 42. CDAC graduate students from the Dlott group at Illinois, Will Shaw and Will Bassett.}
As of May, 2014, 41 graduate students have received the PhD degree, supported fully or in part by CDAC funds to the Academic Partner groups. They are:

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 Velisavljevic (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)
Yu Lin (Stanford, 2012)
Rostislav Hrubiak (Florida International, 2012)
Matt Armentrout (UCLA, 2012)
Walter Uhoya (Alabama-Birmingham, 2013)
Jane Kanitpanyacharoen (UC-Berkeley, 2013)
Jeffrey Finklestein (Princeton, 2013)
Andrew Stemshorn (Alabama-Birmingham, 2014)
Jorge Muñoz (Caltech, 2014)

Figure 43. CDAC graduate student Emma Rainey (UCLA) presenting a talk at the 2013 American Geophysical Union Meeting.
A number of CDAC graduate students have gone on to positions within the NNSA Laboratories or within Department of Energy facilities in general.

### CDAC Students to Postdoctoral Positions at NNSA Labs
- Raja Chellappa
- Wendy Mao
- Nenad Velisavljevic
- Jeffrey Carter
- Kathryn Brown

### CDAC Students to Postdoctoral Positions at Other Federal Government or Government-Supported Labs or Facilities
- James Patterson (WSU Shock Physics)
- Matt Lucas (ORNL)
- Bin Chen (LBL)
- Michael Winterrose (Lincoln Laboratory)
- Wenli Bi (APS, ANL)
- Chris Berg (DOE/BES Office, Washington DC)

### CDAC Students Obtaining Staff Positions at NNSA Labs
- Raja Chellappa (LANL)
- Nenad Velisavljevic (LANL)
- Chris Seagle (SNL)

### Carnegie Postdoctoral Fellows Obtaining Staff Positions at NNSA Labs
- Michael Furlanetto (LANL)
- Amy Lazicki (LLNL)
- Chris Seagle (SNL)
- Luke Shulenberger (SNL)

### Carnegie Postdoctoral Fellows at Other Federal Government Labs or Facilities
- Caitlin Murphy (AIP Congressional Fellow)
- Douglas Allan Dalton (Defense Threat Reduction Agency)

Publications and presentations involving CDAC-supported students and postdoctoral fellows during 2013-2014 are as follows:

### Student Publications
Berg, C., Shock compression and flash-heating of molecular adsorbates on the picosecond time scale, Ph.D. Thesis, University of Illinois at Urbana-Champaign (2014).


Rainey, E. S. G. and A. Kavner, Peak scaling method to measure temperatures to the laser-heated diamond anvil cell and application to the thermal conductivity of MgO, J. Geophys. Res., submitted.


**Student Presentations**


Daviau, K., Preliminary work on the melting of SiC at high pressure, Stewardship Science Academic Programs Symposium (North Bethesda, MD, February 19-20, 2014).


Geballe, Z., S. M. Arveson, S. Speziale, and R. Jeanloz, Sound speed of amorphous CaSiO$_3$ from 0 to 42 GPa, Eos Trans. AGU Fall Meet., Suppl. 94 (2013).

Geballe, Z., Brillouin studies of a highly-stable glass, CaSiO$_3$, from 0 to 44 GPa, Stewardship Science Academic Programs Symposium (North Bethesda, MD, February 19-20, 2014).


Hohensee, G., Metal-diamond interface thermal conductance with nitrogen defects at high pressures by time-domain thermoreflectance, Stewardship Science Academic Programs Symposium (North Bethesda, MD, February 19-20, 2014).


Jugle, M., Deformation and transformation textures in the NaMgF$_3$ perovskite to post-perovskite system, Stewardship Science Academic Programs Symposium (North Bethesda, MD, February 19-20, 2014).


Kaercher, P., Understanding lower mantle rheology from two-phase deformation experiments, Stewardship Science Academic
Lazarz, J., Compression mechanism and equation of state of thaumasite up to 10 GPa, 2013 CDAC Annual Review (Argonne, IL, September 16, 2013).


Lim, J., Origin of pressure-induced volume collapse in Dy, Tb, Gd, and destruction of dense kondo state in CeBa, to 120 GPa, Stewardship Science Academic Programs Symposium (North Bethesda, MD, February 19-20, 2014).


Mauger, L., M. S. Lucas, J. A. Munoz, S. J. Tracy, and B. Fultz, Anharmonic phonon behavior in alpha-Fe at high temperatures, TMS 2013 Neutron and X-Ray Studies of Advanced Materials VI: Centennial and Beyond (San Antonio, TX, March 5, 2013).


Park, S., Complex oxides under extreme conditions of high pressure and irradiation, 2013 CDAC Annual Review (Argonne, IL, September 16, 2013).


Rainey, E., High-pressure thermal conductivity of (Mg,Fe)SiO3 perovskite measured in the laser-heated diamond anvil cell, Stewardship Science Academic Programs Symposium (North Bethesda, MD, February 19-20, 2014).

Rainey, E. and A. Kavner, High-pressure thermal conductivity of (Mg,Fe)SiO₃ perovskite measured in the laser-heated diamond anvil cell, Eos Trans. AGU Fall Meet., Suppl. 94 (2013).


Shelton, H., P. Dera, M. C. Barkley, and R. T. Downs, Phase transition and hydrogen bonding behavior in Be(OH)₂, Zn(OH)₂, and SiO₂ cristobalite at high temperatures and pressures, COMPRES Annual Meeting (Skamania Lodge, WA, June 16-19, 2014).


Stemshorn, A., High pressure high temperature iron-based metallic glass studies, 2013 CDAC Annual Review (Argonne, IL, September 16, 2013).


3.2 Undergraduate Student Summer Scholars

Some of the university students participating in the Carnegie Summer Scholars Program each year carry out their projects in the high pressure group at Carnegie 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 at their home institutions. At Carnegie, such students experience a rigorous introduction to scientific research, and through attendance at CDAC group meetings, are learning about the research process as well as the important problems in the field.

During the summer of 2014, the following students worked with the Carnegie group (Fig. 51). Students funded by CDAC are designated with an asterisk in the list below (*).

**Kevin Hernandez**, California State University-Sacramento  
Reactivity of Hematite and Silica at High Pressure and Temperature

**Olivia Reyes-Becerra**, Stanford University  
Synthesis of Single-Crystal Na₄Si₂₄Clathrate

**Joseph Romero**, Augustana College  
The Effect of Clay on Glycerol/Carboxylic Acid Polymerization

**Brooke Sherman**, George Mason University  
Microbes in the Deep Sea: Analyzing Bacteria from an Inactive Chimney Structure Located Along the East Pacific Rise

**Brandon Wilfong**, Washington College  
In-situ Raman Spectroscopic Investigation of Relaxor Multiferroic Pb(Fe₀.₅Nb₀.₅)O₃ under High Pressure and Temperature Conditions

---

**Figure 51.** Top, Kevin Hernandez, Olivia Reyes-Becerra, and Joseph Romero. Bottom: Brooke Sherman and Brandon Wilfong.
3.3 CDAC Collaborators

The CDAC collaborators from 2013-2014 include the following faculty and students from institutions around the world:

Aarhus Universitet, Denmark
A. Svane

Academy of Science of Moldova
I. M. Tiginyanu
V. V. Ursaki

Air Force Research Laboratory
J. Horwath
S. O. Leontser
M. Lucas
S. L. Semiatin

Ames Laboratory
K. A. Gschneider, Jr.
Y. Mudryk
D. Paudyal
V. K. Pecharsky

Amherst College
D. Ang
J. Gordon
L. Hunter
S. Peck

Aarhus Universitet, Denmark
A. Svane

Argonne National Laboratory
A. Alatas
E. E. Alp
M. Balasubramanian
W. Bi
K. C. Chang
C. C. Chen
P. F. De Carlo
Y. Ding
J. A. Eastman
G. Fabbris
D. D. Fong
P. H. Fuoss
L. Gao
T. Gog
R. Gordon
R. Harder
D. Haskel
S. M. Heald
M. Y. Hu
B. J. Ingram
M. Lerche
W. Liu
J. R. L. Mardegan
D. J. Miller
J. F. Mitchell
E. Perret

Argonne National Laboratory, cont’d
J. A. Schlueter
W. Sturhahn
M. van Veendaal
T. S. Toellner
J. Wen
R. Xu
J. Zhao
H. Zheng
M. Zhernenkov

Arizona State University
D. Benson
G. Farfan
H. Ma
S. H. Shim
Y. Ye

Australian National University
J. E. Bradby
M. W. Doherty
B. Haberl
P. Kluth
N. B. Mason
M. D. Rodriguez
D. J. Sprouster
J. S. Williams

Beijing Computational Science Research Center, China
H. Q. Lin

Beijing University of Technology, China
H. Li
H. Li
X. Zhang

Bhabha Atomic Research Center, India
G. K. Dey
N. Garg
J. Gyanchandani
C. Murli
K. K. Pandey
H. W. Poswal
S. M. Sharma
A. K. Verma

Brookhaven National Laboratory
G. L. Carr
G. D. Gu
X. G. He
W. Ku
T. S. Liu
J. A. Schneeloch
J. S. Wen
Brookhaven National Laboratory cont’d
X. Xi
Z. J. Xu
R. D. Zhong
Calera Corporation
L. Clodic
California Institute of Technology
J. R. Beckett
I. Halevy
S. J. Hwang
J. M. Jackson
Y. Liu
C. Ma
G. R. Rossman
H. L. Smith
J. K. Wicks
Cambridge University, UK
F. Battocchio
Carnegie Mellon University
S. J. Kernion
D. E. Laughlin
A. M. Leary
M. E. McHenry
Case Western Reserve University
Z. Jing
Chinese Academy of Engineering Physics
Q. Wang
X. Wang
Chinese Academy of Sciences
A. Berlie
Y. Bi
X. Dai
L. Deng
Z. Pang
T. D. Hu
F. Huang
F. J. Jia
C. Jin
C. Q. Jin
P. P. Kong
X. Li
Y. Li
C. Lin
C. Q. Lin
T. Lin
J. Liu
L. Liu
Q. Q. Liu
Z. X. Qin
X. C. Wang
Y. Wang
H. M. Weng
G. F. Wu
Chinese Academy of Sciences cont’d
J. J. Wu
T. Xiao
W. Xiao
K. Yang
R. C. Yu
X. H. Yu
Z. Zeng
J. Zhang
J. L. Zhang
S. J. Zhang
Y. S. Zhao
G. H. Zhong
J. Zhu
J. L. Zhu
Civil Aviation University of China
D. An
Z. Li
T. Wei
Q. Zhou
Defense Threat Reduction Agency
D. A. Dalton
Desert Research Institute
H. J. Sun
Deutsches Elektronen-Synchrotron, Germany
H. P. Liermann
Z. Konôpková
A. Rothkirch
Dr. M. V. Shetty Institute of Technology, India
M. R. S. Kumar
École Normale Superieure de Lyon, France
R. Caracas
École Polytechnique Fédérale de Lausanne, Switzerland
H. Berger
Ehime University, Japan
T. Irifune
M. Kimura
I. Ohno
European Synchrotron Radiation Facility, France
W. Crichton
J. Guignard
P. Pattinson
Florida International University
J. Chen
V. Drozd
S. Huang
S. K. Saxena
Keio University, Japan
Y. Kamihara
M. Matoba
A. Wakatsuki
Korea Advanced Institute of Science and Technology
M. J. Han
H. S. Kim
KTH Royal Institute of Technology, Sweden
A. B. Belonoshki
Kurchatov Institute, Russia
V. V. Roddatis
Lawrence Berkeley National Laboratory
B. Chen
T. Cuk
J. Knight
A. MacDowell
D. Y. Parkinson
J. Yan
Lawrence Livermore National Laboratory
C. Aracne-Ruddle
S. Bonev
J. A. Bradley
K. Catalli
J. Y. Chen
H. Cynn
W. J. Evans
J. R. Jeffries
Z. Jenei
A. Landa
M. J. Lipp
D. Ruddle
P. Soderlind
S. T. Weir
K. Visbeck
Lehigh University
K. Landskron
M. Mandal
Los Alamos National Laboratory
M. M. Bishop
P. R Bowden
R. S. Chellappa
J. D. Coe
L. Daemen
D. M. Dattelbaum
N. H. Mack
V. W. Manner
D. N. Preston
Z. Quan
R. Saavedra

Los Alamos National Laboratory, cont’d
L. L. Stevens
J. D. Thompson
N. Velisavljevic
Massachusetts Institute of Technology
P. N. Chen
C. Gu
Max Planck Institut für Chemie, Germany
M. Eremets
T. Palasyuk
I. Troyan
H. Wang
Max Planck Institut für Chemische Physik fester Stoffe, Germany
S. Medvedev
Max Planck Institut für Festkörperforschung, Germany
A. Yaresko
McMaster University, Canada
G. A. Bottom
S. Prabhudev
National Academy of Science, Ukraine
Y. A. Freiman
A. Grechnev
S. M. Tretyak
National Center for Nanoscience and Technology, China
M. He
National Chiao Tung University, Taiwan
Y. C. Tseng
National Energy Technology Laboratory
R. R. Ohodnicki
National Institute of Standards and Technology
P. M. Gehring
Naval Research Laboratory
N. Bernstein
J. L. Feldman
New Jersey Institute of Technology
E. L. Dreizin
R. A. Williams
Northern Illinois University
O. Chmaissem
Northwestern University
J. W. Doak
A. Issa
S. J. Kirklin
X. Liu
M. Merino
S. M. Thomas
C. Wolverton
Oak Ridge National Laboratory
D. L. Abernathy
I. I. Al-Qasir
Y. Q. Cheng
O. Delaire
A. M. dos Santos
R. S. Fishman
K. Gofryk
I. N. Ivanov
J. Ma
M. E. Manley
J. J. Molaison
N. Pradhan
B. C. Sales
A. S. Sefat
D. J. Singh
M. B. Stone
C. A. Tulk

Oakland University
I. Efthimiopoulos
J. Kemichick
M. Kucway
Y. Wang

Ohio State University
J. E. Kabbes
W. Panero
J. S. Pigott

Osaka University, Japan
Y. Nakamoto
K. Shimizu

Pacific Northwest National Laboratory
M. E. Bowdren

Paul Scherrer Institute, Switzerland
R. Dähn
D. Gromilund
P. Schaub
E. Wieland

Peking University
T. Gu
S. Qin
R. Tao
X. Wu
L. Zhang

Polish Academy of Sciences, Poland
E. Magos-Palasyuk
P. Zaleski-Ejgierd

Poly Crystallography Inc.
J. A. Kaduk

Princeton University
H. Dong
S. M. Dorfman
T. S. Duffy
G. J. Finkelstein

Princeton University, cont’d
D. He
C. M. Holl

Rensselaer Polytechnic Institute
H. C. Watson

Russian Academy of Sciences
F. S. Elkin
A. G. Gavriliuk
A. G. Ivanova
S. S. Khasanov
K. D. Litasov
I. S. Lyubutin
A. A. Mironovich
P. G. Naumov
A. P. Novikov
S. G. Ovchinnikov
A. E. Petrova
Y. A. Sidorov
S. M. Stishov
A. L. Vasiliev
I. P. Zibrov

Sandia National Laboratory
C. Seagle

Santa Clara University
H. Lee
A. Zabelegui

Savannah River National Laboratory
D. A. Knight
R. Lascola
R. Zidan

Seoul National University, Korea
S. K. Lee

Shandong University, China
J. Fan
H. Jiang
X. Tao

Sichuan University, China
S. N. Luo

SLAC National Accelerator Laboratory
T. P. Devereaux
A. F. Kemper

Smithsonian Institution
B. Grocholski

South China University of Technology
Q. W. Huang
S. Jiang
J. Liu
Z. X. Qin
L. Y. Tang
J. Zhang
J. B. Zhang
Z. B. Zhang
X. M. Zhao
Southern University
S. Yang
SPring-8, Japan
T. Ishikawa
Y. Kohmura
C. Song
Stanford University
J. C. Andrews
E. Boulard
R. M. K. Carlson
J. E. P. Dahl
G. A. Farfan
I. R. Fisher
T. Geballe
A. Gleason
S. Hirai
Y. Lin
Y. Liu
W. L. Mao
S. C. Riggs
M. C. Shapiro
Z. X. Shen
C. V. Shi
S. Wang
F. Yang
Q. Zeng
Z. Zeng
H. Zhang
Z. Zhao
State University of New York - Sony Brook
S. E. Boulfelfel
P. Chen
Z. Chen
X. G. Hong
B. Li
W. Liu
A. O. Lyakhov
M. Ma
A. R. Oganov
L. B. Skinner
D. Xu
W. Zhang
Q. Zhu
Stockholm University, Sweden
L. Eriksson
U. Haussermann
J. Nylen
Swiss Light Source
F. Marone
R. Mokso
M. Stramanoni
Synchrotron SOLEIL, France
N. Guignot
Tata Institute of Fundamental Research, India
A. Thamizhavel
Technische Universität Darmstadt, Germany
C. Trautmann
Tohoku University, Japan
M. W. Chen
T. Sakamaki
A. Suzuki
Tokyo Institute of Technology, Japan
M. Azuma
Toyota Research Institute of North America
C. Ling
R. Mohtadi
P. Sivasubramanian
Tsinghua University, China
H. Gong
L. Li
X. Wang
S. Zhang
Unità Tecnica Caratterizzazione, Italy
A. R. Sprocati
F. Tasso
United States Army Research Laboratory
D. M. Reaman
Universidad de Los Andes, Colombia
R. S. McWilliams
Universidade Estadual de Campinas, Brazil
C. Giles
J. R. L. Mardegan
L. S. I. Veiga
Universidade Federal do ABC, Brazil
M. Avila
Universität Augsburg, Germany
J. Deisenhofer
A. Loidl
V. Tsurkan
Universität Bayreuth, Germany
D. J. Frost
T. Katsura
C. A. McCammon
Universität Bern, Switzerland
A. Jenni
U. Mäder
Universität Bremen, Germany
R. X. Fisher
H. Lührs
H. Schneider
3.4 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.

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Experiment Description</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>A. Palke</td>
<td>Stanford University</td>
<td>Ferric-iron perovskite synthesis with Yingwei Fei</td>
<td>January 7-28, 2013</td>
</tr>
<tr>
<td>E. J. Kim</td>
<td>Seoul National University</td>
<td>High pressure samples of silicates with CO₂ with Yingwei Fei</td>
<td>January 21-25, 2013</td>
</tr>
<tr>
<td>J. Wu</td>
<td>University of Texas at Austin</td>
<td>Experiments for superconductors with Viktor Struzhkin</td>
<td>January 21-25, 2013</td>
</tr>
<tr>
<td>K. Post</td>
<td>University of California – San Diego</td>
<td>High pressure measurements of intermetallic compounds</td>
<td>January 30-February 8, 2013</td>
</tr>
<tr>
<td>D. Wai</td>
<td>Shanghai Jiaotong University</td>
<td>Computational physics of materials and high-pressure Fe-S with Yingwei Fei</td>
<td>February 19-March 1, 2013</td>
</tr>
<tr>
<td>T. Zapata</td>
<td>Texas A&amp;M University</td>
<td>Materials under high pressure using a DAC with Viktor Struzhkin</td>
<td>February 18-22, 2013</td>
</tr>
<tr>
<td>R. Chellappa</td>
<td>LANL</td>
<td>Work with Maddury Somayazulu</td>
<td>February 26-March 2, 2013</td>
</tr>
<tr>
<td>S. Starchikov</td>
<td>Institute of Crystallography, RAS</td>
<td>DAC experiments with Viktor Struzhkin</td>
<td>March 18-31, 2013</td>
</tr>
<tr>
<td>C. Ji</td>
<td>ANL</td>
<td>Sample loading with Ho-kwang Mao</td>
<td>March 18-22, 2013</td>
</tr>
<tr>
<td>L. Gasparov</td>
<td>University of North Florida</td>
<td>High pressure study of magnetite with Viktor Struzhkin</td>
<td>April 29-May 10, 2013</td>
</tr>
<tr>
<td>N. Timmins</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F. Huang</td>
<td>Johns Hopkins University</td>
<td>High P-T experiments with Yingwei Fei</td>
<td>May 21-August 20, 2013</td>
</tr>
<tr>
<td>R. Caracas</td>
<td>Ecole Normale Superieure de Lyon</td>
<td>Work on carbonatite melts with Ronald E. Cohen</td>
<td>June 3-7, 2013</td>
</tr>
<tr>
<td>R. Boles</td>
<td>University of Nevada – Reno</td>
<td>Properties of amorphous metal ribbons at high pressures with Maddury Somayazulu</td>
<td>June 10-28, 2013</td>
</tr>
<tr>
<td>J. Holaday</td>
<td>Walt Whitman High School</td>
<td>High pressure synthesis experiments with Timothy Strobel</td>
<td>June 24-August 25, 2013</td>
</tr>
<tr>
<td>W. Grochala</td>
<td>University of Warsaw</td>
<td>High pressure conductivity studies of AgF₂ and AgF₆; Transport optical measurements with Viktor Struzhkin</td>
<td>June 24-July 5, 2013</td>
</tr>
<tr>
<td>C. Tulk</td>
<td>Oak Ridge National Laboratory</td>
<td>Work with Maddury Somayazulu</td>
<td>August 12-14, 2013</td>
</tr>
<tr>
<td>Y. Davyolova</td>
<td>Moscow Engineering Physics Institute</td>
<td>High pressure optical experiments with Viktor Struzhkin</td>
<td>September 17-October 17, 2013</td>
</tr>
<tr>
<td>A. Kyono</td>
<td>University of Tsukuba</td>
<td>Single crystal XRD experiments with Timothy Strobel and Stephen Gramsch</td>
<td>September 18-24, 2013</td>
</tr>
</tbody>
</table>
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<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Research Description</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>N. Holtgrew</td>
<td>Howard University</td>
<td>Laser optics in Raman pump-probe experiments with Alexander Goncharov</td>
<td>October 1, 2013-September 30, 2014</td>
</tr>
<tr>
<td>S. Cervera</td>
<td>University of Paris</td>
<td>Measurements of elasticity of Fe by an ultrafast laser pump-probe technique with Alexander Goncharov</td>
<td>November 18-29, 2013</td>
</tr>
<tr>
<td>Z. Konopkova</td>
<td>DESY</td>
<td>Resolved laser heating of samples under pressure with Alexander Goncharov</td>
<td>February 18-June 30, 2014</td>
</tr>
<tr>
<td>D. Keefer</td>
<td>Pennsylvania State University</td>
<td>High pressure work with Timothy Strobel</td>
<td>February 18-21, 2014</td>
</tr>
<tr>
<td>E. Monroe</td>
<td>Woodrow Wilson Senior High School</td>
<td>Studies of NV centers in diamond under compression with Viktor Struzhkin</td>
<td>July 15-August 15, 2014</td>
</tr>
</tbody>
</table>

3.5 2013 and 2014 SSAA Symposia

The 2013 SSAA Program Symposium took place in Albuquerque, NM on June 27-28 (Fig. 52), and in 2014, the Symposium was held in North Bethesda, MD on February 19-20 (Fig. 4). At both meetings, individual grant recipients and center directors from the three divisions of the program (High Energy Density Physics, Low Energy Nuclear Science, and Materials Properties under Extreme Conditions) gave updates on center or group activities and progress.

In 2013, the symposium was opened with a welcome address from Ralph Schneider, the Director of the Office of Defense Science at the NNSA. Paul Hommert, Director of Sandia National Laboratories, gave the keynote talk before the poster session. CDAC students and partners were joined by two CDAC and HPCAT scientists and presented 18 posters during the poster session on the first night of the symposium. CDAC Director Russell Hemley gave two invited talks, one an overview of CDAC and one with Yogendra Gupta (Washington State University) on unique opportunities at the APS, featuring HPCAT and DCS. CDAC Students Pamela Kaercher (Berkeley), Zeyu Li (Michigan), Lisa Mauger (Caltech), and Eloisa Zepeda-Alarcon (Berkeley) all received Best Poster awards during the poster session. This was the second year in a row that Pamela earned this honor.

In 2014, the Symposium was held in North Bethesda, MD from February 19-20, 2014. The symposium was opened with a welcome address from Keith LeChien, the Program Manager in the Defense Science Division at the NNSA. Bruce Held, Acting Administrator (NNSA) and Acting Undersecretary for Nuclear Security (DOE), gave the keynote talk before the poster session. CDAC students and scientists presented 18 posters during the poster session. In addition, CDAC

![Figure 52. CDAC graduate students Sulgiye Park (Michigan) and Lisa Mauger (Caltech) with their posters at the 2013 SSAP Symposium in Albuquerque, NM.](image-url)
Director Russell Hemley gave an invited talk, presenting an overview of CDAC. CDAC Students Pamela Kaercher (Berkeley), Emma Rainey (UCLA), and Dane Tomasino (WSU) all received Best Poster awards during the poster session. Pamela received a Best Poster award for the third consecutive year.

**CDAC Posters Presented at the 2013 SSAA Program Symposium**


**CDAC Posters Presented at the 2014 SSAA Program Symposium**


Daviau, K., Preliminary work on the melting of SiC at high pressure, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).


Uhoya, W., High pressure effects on the superconductivity in rare earth doped CaFe₅As₂, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).


### 3.6 Paris-Edinburgh Cell Workshop

The CDAC-supported *Paris-Edinburgh Cell Workshop 2013* was held on May 23-24 at the APS and HPCAT 16BM-B, (Fig. 53). More than 45 participants attended the two-day workshop. The workshop was composed of four technical training courses, as well as a discussion forum related to current Paris-Edinburgh cell applications in high-pressure research. 32 graduate students, postdocs, and young and senior researchers, among the participants who had little to no experience with Paris-Edinburgh (PE) cell applications, took hands-on courses. This training included instruction in a standard sample cell assembly (established for HPCAT PE cell application), high *P-T* control, ultrasonic measurement, and EDXD data analysis. A falling sphere viscometry technique was also demonstrated. The unique opportunity provided by the new instrumental setup established at HPCAT was also introduced to the hands-on participants through these courses. The workshop, which was organized by HPCAT's Changyong

*Figure 53. Paul Chow discusses x-ray spectroscopy as part of a tour of HPCAT at the Paris-Edinburgh Cell Workshop.*

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Park, Yoshio Kono, and Guoyin Shen (HPCAT), along with Yanbin Wang from GSECARS, was a successful outreach to the potential user community.

3.7 CDAC Year 11 Review

On September 16-17, 2013, CDAC hosted its Year 11 Review at the Advanced Photon Source at ANL (Fig. 54). In addition to a program overview by Director Russell Hemley, and a presentation on education and outreach activities by Coordinator Stephen Gramsch, HPCAT Director Guoyin Shen also provided an update on HPCAT capabilities and an overview of the APS and HPCAT upgrade plans. Ten of the Academic Partners also made presentations to the review committee. The presentations from the partners included six continuing partners and four new partners that joined the program in 2013. Nenad Velisavljevic (LANL) and Chris Seagle (SNL), two former CDAC students who now hold staff positions in the NNSA Labs, also made presentations on the work that they have carried out with CDAC beam time. The poster session included presentations by 16 current and former CDAC students.

**Monday, September 16, 2013:**
- 8:00-8:30 Review Committee Executive Session
- 8:30-9:15 Russell Hemley – Overview
- 9:15-9:45 Steve Gramsch – Education and Outreach
- 9:45-10:15 Guoyin Shen – Update on HPCAT Capabilities
- 10:30-11:00 Dana Dlott – University of Illinois
- 11:00-11:30 Yogesh Vohra – University of Alabama-Birmingham
- 11:30-12:00 Jim Schilling – Washington University in St. Louis
- 12:00-12:30 Abby Kavner – University of California-Los Angeles
- 12:30-2:30 Lunch and Student Poster Session
- 2:30-3:00 Steve Jacobsen – Northwestern University
- 3:00-3:30 David Cahill – University of Illinois
- 3:30-4:00 Nenad Velisavljevic – Los Alamos National Laboratory
- 4:00-4:30 Chris Seagle – Sandia National Laboratories
- 4:30-5:00 Review Committee Executive Session

**Tuesday, September 17, 2013:**
- 8:30-9:00 Eva Zurek – University at Buffalo
- 9:00-9:30 Lowell Miyagi – University of Utah
- 9:30-10:00 Choong-shik Yoo – Washington State University
- 10:00-10:30 Przemek Dera – University of Hawai‘i
- 10:30-10:45 Russell Hemley – Summary
- 11:00-11:30 Tour of HPCAT
- 11:30-12:00 Review Committee Meeting
- 12:00-12:30 Review Committee Executive Session

*Posters Presented at the CDAC Review*

- Bi, W., Applications of nuclear resonant scattering in high pressure research at Sector 3 of the Advanced Photon Source, 2013 CDAC Annual Review (Argonne, IL, September 16, 2013).
- Lazarz, J., Compression mechanism and equation of state of thauamasisite up to 10 GPa, 2013 CDAC Annual Review (Argonne, IL, September 16, 2013).


### 3.8 USA Science and Engineering Festival

Carnegie Postdoctoral Fellow Caitlin Murphy was among a number of Carnegie scientists participating in the third annual USA Science and Engineering Festival, held at the Washington Convention Center in Washington, DC, from April 26-27, 2014 (Fig. 5). This is the largest science, technology, engineering, and math education event of its kind in the US. Caitlin presented a demonstration on her topic, "How does high pressure affect materials that have defects and impurities?" Robert Hanrahan, former Program Manager for CDAC at NNSA, discussed stockpile stewardship and non-proliferation at the State Department's booth in the National Security Section of the event.

### 3.9 2014 Neutron and X-ray Scattering School

HPCAT Beamline Scientists Changyong Park and Dmitry Popov hosted a group of eight graduate students during the 2014 Neutron and X-ray School. The NX School was held on June 19-20 at the APS. During the two-day class, HPCAT 16-BM-D hosted groups of students who learned about XRD with hands-on training for high-pressure experiments using the DAC and received a practical introduction to data analysis.

### 3.10 Honors and Awards

CDAC Academic Partner Steven Jacobsen from Northwestern received a Friedrich Wilhelm Bessel Research Award for 2014. The Bessel Award is granted by the Alexander von
Humboldt Foundation, and allows the recipient to spend a year working at a research institution in Germany. He will spend the coming year at the Bayerisches Geoinstitut in Bayreuth, where he was a Humboldt Postdoctoral Fellow from 2002-2004. Eva Zurek, a CDAC Academic Partner from the University at Buffalo, received the 2014 Young Leaders Professional Development Award of The Minerals, Metals and Materials Society (TMS). She was presented with the award at the 2014 annual meeting of the TMS in San Diego, CA.

CDAC Partners Przemek Dera (University of Hawai'i) and Lowell Miyagi (University of Utah) have been named as the speakers for the 2014-2015 COMPRES Distinguished Lecture series in the field of Mineral Physics. The talks feature topics that emphasize the exciting high-pressure geoscience research being conducted within the COMPRES community and its significance for understanding fundamental Earth and planetary processes. Since its inception in 2008, seven CDAC Academic Partners and/or faculty who were supported as postdoctoral fellows through CDAC have served as Distinguished Lecturers.

4. TECHNOLOGY DEVELOPMENT

Technical development remains an important focus area in CDAC. At HPCAT, NSLS and in the Academic Partner groups, an ongoing significant effort in this area has resulted in many breakthroughs in measurement capabilities, which enable the cutting edge science pursued across the Center. In this section, we outline some of the technology development efforts that have taken place in the Center during 2013-2014.

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. 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. Over the past year, each of the beamlines at HPCAT has undergone significant improvements in capabilities and performance.

16-ID-D: High Pressure X-ray Spectroscopy – HPCAT beamline 16-ID-D specializes in hard x-ray spectroscopy experiments with samples under high pressure in DACs. In the current configuration, three types of measurements can now be carried out: nuclear forward/nuclear resonant inelastic scattering, x-ray resonant/non-resonant emission and energy loss spectroscopy with 1.4 eV energy resolution. 16-ID-D is one branch of a canted line, with a 3.0 mm period APS undulator and a liquid nitrogen-cooled Si(111) high heat load monochromator delivering x-ray energies of 4.5-37 keV. Several combinations of focusing mirrors are used for various needs in user operation. Typically for flux hungry measurements, the beamline features 1-meter long vertical and horizontal mirrors to achieve 35µV x 55µH focus size at the sample position. For a smaller beam at the expense of incoming flux, the setup consists of a pair of 200 mm mirrors for a 3µV x 5µH focus. A combination of one short and one long mirror may be used for special geometries.

In the past year, a number of development projects and improvements have been made to enhance the performance of the beamline and extend its capabilities.
• Working with the APS, design and testing of a pre-figured mirror, to focus the beam suitable for megabar pressures, has begun.
• A multiple-analyzer emission spectrometer is in the final construction stage, and will increase the efficiency of data collection by a factor of 7.
• A low-momentum transfer, 100 meV resolution energy-loss x-ray spectrometer is under commissioning for the study of collective and single particle electronic excitations.
• Automated beamline control software has been progressively upgraded to PyEpics standards. This will allow users the flexibility and ease of writing scripts for various purposes, including data collections and evaluations. The recently installed quad-diode beam position monitor and feedback software ensures a stable beam position, and optimizes the intensity of the beam on the sample (Fig. 57).

16-ID-B: General Purpose Microdiffraction – 16-ID-B is an undulator beamline dedicated to x-ray microdiffraction over a vast range of pressure and temperature conditions. The General Purpose (GP) Table is one of two measurement stations in the experimental hutch and is optimized to handle various types of diffraction experiments (single-crystal and powder) over broad pressure and temperature ranges (ambient pressure to several hundred GPa and ~4 to 1,000 K) with DACs in axial or radial geometry. Continual development at the GP Table makes it a highly productive, high-throughput beamline.

The 200 mm Pt-coated focusing mirrors have been upgraded to 320 mm Pt/Rh-coated mirrors. This combination of increased length and coating yields an increase in flux by about a factor of five. Also, the robust mechanical design offers a more stable beam position and focal spot size. Mirrors, sample, and detector have been mounted on a common table which, in turn, has been stabilized by decoupling it from its translation mechanisms when not in use. This has resulted in an extremely stable experimental configuration that can remain internally stable to within the repeatability of the mechanical stages (micron level) even after displacement of a large mass (~50 kg) across the optical table.

Specialized developments at the GP table are also focused on the emerging field of time-resolved diffraction. Now, timing electronics and pressure control (pneumatic membrane or piezoelectric stack) can be remotely and conveniently controlled using a GUI from the control station. High-frequency (125 Hz) diffraction imaging can be synchronized with ramp compression or stroboscopic pressure cycling using an arbitrary-wave function generator and an 8-channel delay generator. Rapid on-line data analysis has been achieved through optimizing existing software (e.g., batch processing of thousands of images and diffraction patterns) to generate high-quality pressure-temperature-volume relations. One highlight was the recent test of an area detector prototype with imaging capability of 800 Hz, allowing the demonstration of compression rates exceeding tens TPa/s (Fig. 10).

16-ID-B: Microdiffraction with Double-Sided Laser Heating – The laser heating table at HPCAT is heavily used during each run cycle, and the apparatus undergoes continuous improvement in response to the needs of many users (Fig. 58). Recent developments on the laser heating table include:
• *In-situ* variation of the laser heating spot size allows changing the heating spot size anytime as needed, even during heating. This is an effective way to eliminate or minimize the effect of temperature gradients on samples, especially those with complex chemistry. The alignment of
laser and x-ray beams to one spot on sample and maintaining the alignment during an experiment are critical for obtaining meaningful and reliable data. As sample size getting smaller to micron level, maintaining the alignment becomes more challenging.

- Laser power can now be modulated into short pulses or various ramp (up or down) paths and synchronized with diffraction and temperature measurements. This capability is a useful tool for studies of high-pressure melting phenomena and also enables time-resolved studies.
- The capability to synchronize the XRD measurement at 500 ns exposure with the APS hybrid singlet mode (8 groups of 7 consecutive bunches in 500 ns) has been established. This capability can be used for time-resolved and pump-probe studies.
- Synchronized laser pulse with thermal imaging allows for monitoring the temperature distribution on samples during pulsed laser heating experiments. The setup allows the recording of thermal images from the heated samples with exposure times down to 1 μs, which is crucial for controlling the sample heating, temperature homogeneity and position alignment in time-resolved experiments.

16-BM-D: X-ray Absorption and Microdiffraction – With the commissioning of x-ray absorption techniques at 16-BM-D, this station has become heavily subscribed for a variety of challenging measurements at high pressure. Important new developments at 16-ID-B include the following.

A Perkin-Elmer amorphous Si pixel array detector (2048 × 2048 pixels with 200 μm fixed size) at the 16-BM-D station now readily achieves high-resolution XRD at the level of Δq/q ~ 2.5×10-3 angular resolution as a result of locating the detector at a large sample-to-detector distance (up to ~900 mm). The new instrumental setup substantially reduces the data acquisition and reduction time.

Figure 59. Interchangeable micro-XRD (left) and XANES (right) setup at 16-BM-D provides a simultaneous probe of atomic and electronic structure at the same sample conditions.
The XANES measurement has been newly introduced for the 16-BM-D station. The focused (4-5 µm horizontal and 12-15 µm vertical) monochromatic x-ray beam, for which the energy is determined by a Si (111) double crystal monochromator in pseudo-channel cut mode, is delivered to the sample stage with minimal offset of beam height (~2 µm per 1 keV scan range). The capability of performing an energy scan while keeping the finest focus of beam at the sample enables conducting the XANES measurement with DAC samples. The capability of high-energy XANES measurements for K-edge absorption spectroscopy of heavy elements (e.g., Ce K absorption edge at 40.443 keV) is unique to 16-BM-D compared to other stations. The ion-chamber detectors for the XANES measurement are mounted on an in-and-out type pneumatic stage, which is fully compatible with the standard XRD setup at 16-BM-D, so that the XANES measurement can be easily combined with high-resolution XRD measurements without disturbing the sample (Fig. 59).

**16-BM-B: White-Beam Laue Diffraction** – Currently, the white beam diffraction setup is under commissioning at 16-BM-B. This is intended for time resolved studies of crystal lattice defects and deformation *in situ* under external stress. Potential areas of application may include studies of mechanisms defining kinetics of pressure-induced phase transitions or phase transformations under high pressure such as melting or crystal growth, mechanisms of deformation, and shock compression.

Over the past year some measurements on single crystals during pressure induced phase transitions have been performed. For example, spatially resolved white beam Laue data from Si during the α-β phase transition have been obtained. A series of consecutive 2D translational scans have been collected on a Si single crystal until the phase transition was completed. The alteration due to the phase transition was indicated by the appearance of additional diffuse reflections, and at the same time the original single crystal of α-Si exhibited splitting into distorted blocks (Fig. 60). The altered areas have been located right between the blocks of the α-phase.

Improvements in the data reduction process have focused on the development of an approach to quantify crystal lattice rotations. Precision better than 0.05° was obtained from one diffraction pattern typically collected in 0.5 seconds of exposure. Important to note is the fact that such a measurement with a monochromatic beam would require fine angular slicing and it would take at least tens of seconds to get enough data. Total data collection time would be 1-2 orders of magnitude longer than with the Laue technique, and even then most of the observed changes during the studied phase transitions would not be identified.

![Figure 60. Left: Si single crystal at pressure right above the α-β phase transition. Center: composite frame of the (862) reflection of α-Si. Right: composite frame of diffuse reflection from the altered area. Red frames on the center and right images reproduce the shape of the original sample.](image-url)
**16-BM-D: Paris-Edinburgh Cell Program** – Techniques for measuring liquid structure, elastic wave velocity, and viscosity under high pressure have been optimized for the Paris-Edinburgh cell at 16-BM-B. The Paris-Edinburgh press allows for compressing large volume samples (up to 2 mm in both diameter and thickness) up to ~7 GPa and 2000 °C.

Ongoing development for anvil and cell design recently enabled measurements at up to ~12 GPa and 1800 °C. Multi-angle energy dispersive XRD provides structure factors of liquids to a large Q of ~20 Å⁻¹. Ultrasonic techniques have been developed to investigate elastic wave velocities of amorphous solids and liquids combined with the x-ray imaging. Falling sphere viscometry, using high-speed x-ray imaging (>1000 frames/second), enables investigations over a wide range of viscosity, from those of high viscosity silicate or oxide melts to low viscosity (<1 mPa s) liquids and fluids such as liquid metals or salts. The integration of these multiple techniques has promoted comprehensive studies of structure and physical properties of liquids as well as amorphous materials at high pressures and high temperatures, making it possible to investigate correlations between structure and physical properties of liquids and amorphous solids.

This phase contrast imaging setup has allowed observations of the behavior of low density contrast liquids such as water and oil, which will eventually enable studies of phase separation and liquid-liquid immiscibility at high pressures and high temperatures.

Preliminary experiments with the dynamic DAC were conducted for water by optical imaging (Fig. 61). The sample was rapidly decompressed, and high-speed optical imaging (5000 frames/second) successfully monitored the melting behavior of water, and subsequent falling of a ruby ball in water, which provides important information for determining viscosity. High-speed x-ray imaging allows observations of not only optically transparent materials but also opaque materials such as liquid metals. The combination of high-speed x-ray imaging and the dynamic DAC opens up new techniques for studying the nature of melting/crystallization and the behavior of liquids at high pressures.

**Supporting Facilities at HPCAT** – Ancillary capabilities at HPCAT are crucial to the success of the overall experimental program, and all personnel dedicate significant effort to improve these facilities on an ongoing basis to expand the available P-T range of the experimental conditions, increase efficiency and productivity of the beamlines, improve the quality of experimental data, and integrate additional methods of sample characterization with synchrotron investigations.

In order to fully utilize remote pressure control capabilities, a number of portable online optical systems for ruby fluorescence pressure measurements and in-situ Raman sample characterization have been designed. Now, online optical systems are available for every experimental station at HPCAT. Combined with remote pressure control systems, they significantly increase the productivity of beamlines during high-pressure experiments.

Techniques and instrumentation have been developed for collecting high-quality, time-resolved x-ray scattering data and bridging the gap between static and dynamic high-pressure measurements by enabling rapid controlled uni- and bi-directional or cyclic sample compression/decompression up to extreme compression rates in excess of a TPa per second. These time-resolved

![Figure 61. a) High-speed imaging of the melting of water. b) Subsequent falling of a ruby sphere in water.](image-url)
techniques are currently used for synthesis/observation of metastable high pressure phases, and studying phase transition kinetics and fast rheology.

Because sample quality is a major factor in success of any experiment, HPCAT has established state-of-the-art sample preparation and characterization facilities, which include numerous modern microscopes, a glovebox, sample polishing facilities, a laser drilling and micromachining unit, and offline laser heating and Raman systems.

4.2 HPCAT-CDAC Collaborations

High Pressure Mineral-Fluid Interface Cell – The electron density profile of a mineral-water interface and the element-specific sub-profile can be measured with synchrotron-based high-resolution x-ray reflectivity (HRXR) and resonant anomalous x-ray reflectivity (RAXR) techniques, and it has been known that the interfacial structure and processes are highly specific to the system due to inherent complexity of solid surface. The convoluted effects of a surface termination, morphology, chemistry, and charge distribution typically result in a unique interfacial profile and process for each individual system. However, the experimental approaches with HRXR and RAXR have been limited to the sample conditions only with ambient pressure and temperatures lower than 100 °C due to limited sample cell capabilities, which in turn limits the utilization of the experimental techniques only to non-hydrothermal systems. To overcome this limitation, Changyong Park at Carnegie has developed a high P-T aqueous interface cell that can maintain static pressure and temperature conditions up to 40 MPa and 500 °C (Fig. 62). Pilot tests of the new cell and the preliminary applications to the olivine (010)-water interface have been made at HPCAT ID-D and APS Sector 5-ID-C.

High P-T Thermal Measurements in the Paris-Edinburgh Cell – Discretionary CDAC beam time was utilized the development of simultaneous XRD, x-ray radiography, electrical resistance, and thermal measurements with the Paris-Edinburgh (PE) cell. Laboratory Partner Nenad Velsavljevic (LANL) and student Jason Baker collaborated with Ravi Kumar (UNLV), Changyong Park to improve the experimental setup and establish the feasibility of performing the

**Figure 62.** Schematic diagram of the pressure, temperature and flow rate control of the high pressure mineral-fluid interface cell.

**Fig. 63.** Left, Variation in electrical resistance in Bi during isothermal (298 K) compression as the sample undergoes the I→II→II structural transitions. Right, isobaric (2.2 GPa) heating results in a gradual change in electrical resistance as the sample undergoes the I→II transition.
combined measurements with PE cell. Preliminary measurements were performed on Bi metal and feasibility was demonstrated up to ~6 GPa and ~1000°C (Fig. 63).

**A New Furnace for High-Temperature NRIXS Measurements** – Graduate student Lisa Mauger, from the Fultz group at Caltech, has developed a specialized furnace that can be interfaced to beamline 16-ID-D at HPCAT to carry out NRIXS measurements at elevated temperatures (Fig. 46). The work was carried out in collaboration with former CDAC student Matt Lucas at the Air Force Research Laboratory.

### 4.3 Frontier Synchrotron Infrared Spectroscopy under Extreme Conditions

The Frontier Synchrotron Infrared Spectroscopy (FIS) Beamline for Extreme Conditions has been approved as one of the eight NxtGen beamlines to be developed and constructed at NSLS-II. FIS is the successor of the IR-DAC facility (U2A) at NSLS, the highly productive, Carnegie-managed user facility supported by COMPRES and CDAC, and the only dedicated high-pressure synchrotron IR facility in the world.

As announced in May 2012 at the NSLS/CFN Joint Users’ Meeting by Dr. Steve Dierker, Associate Laboratory Director for Photon Sciences, NxtGen is a set of eight beamlines at NSLS-II that will be based on components from beamlines at NSLS. Carnegie’s Zhenxian Liu and Russell Hemley and the FIS team have been working closely with the BNL Photon Sciences staff to move forward with the development of FIS. A Beamline Execution Plan detailing the FIS project is in the advanced draft stage. FIS will adapt one of the novel design features of NSLS II – the large-gap IR dipole. Construction of the beamline hutch on Bending Magnet Port 22 will be completed and all existing equipment at U2A moved in by early 2015. At that time, the integrated optical facility for far-IR to UV absorption and reflectance spectroscopy with conventional sources, together with laser Raman and photoluminescence spectroscopy will open to users for experiments – i.e., during the NSLS/NSLS-II “dark period.” Full synchrotron IR capability will be available no later than 2017, with early completion anticipated pending efforts to obtain supplemental funding.

The FIS beamline will enable in-situ optical studies of a wide variety of materials by spectroscopic techniques at extreme $P-T$ conditions, from ambient to several megabars, and from 4-6000 K. Measurements from the far-infrared to visible range will be possible with diffraction-limited resolution. The combination of the high brightness and low noise of NSLS-II with dedicated high-pressure facilities will be unique in the world.

### 4.4 Technique Development at Carnegie

**Melting of Refractory Transition Metals** – The mechanical strength of materials is known to decrease drastically at temperatures as low as half of their melting points, and the melting behavior of various metals has shown a large variation in their dependence on stress. The direct and accurate measurement of melting temperatures of these metals under extreme stress is therefore not only imperative in understanding the fundamentals of melting but also important.

![Figure 64. SEM photos of laser-heated spots at 3538 K (a, b) and 4326 K (c, d) on the Re sample recovered from 22 GPa. Surfaces are shown in (a, c), and cross sections through the laser heated spots are shown in (b, d). Recrystallization to sub-µm depth with no change in textural appearance is evident in (b), compared with the unheated portion. Complete restructuring of the metal with a sharp boundary to a depth of several µm between the quenched liquid and the unmolten sample is shown in (d).](image)
for synthesizing new strong materials. Measuring melting under high pressure is challenging, however. Typical notorious problems associated with prolonged measurements (a few seconds) in a LHDAC are chemical reactions, sample instability and thermal runaway, while using too short a laser heating time (~μs) increases temperature uncertainty. To address these problems, Carnegie’s Reinhard Boehler and graduate student Amol Karandikar have developed a new “flash heating” method for melting studies at high pressure in the LHDAC.\(^{53}\)

Polished metallic samples (50-60μm diameter, 8-10μm thick) are loaded in the DAC in an inert argon pressure medium that also provides thermal insulation from the diamond on the side to be heated. A heating laser (1070 nm) is aligned with an optical setup for measuring temperatures. The sample is heated with a 20 ms rectangular laser pulse, and the thermal response is monitored with a fast photomultiplier while measuring the steady state temperature with a CCD spectrometer. The 20 ms pulse is long enough to measure the temperature reliably and short enough to avoid any chemical reaction and thermal instabilities in the sample. For each new unheated area on the sample, the laser power is increased to produce a temperature rise of ~100 K. Typically, one sample disc is sufficient for 8-10 heated spots while recording both temperatures and locations.

Samples are then recovered to ambient conditions and are analyzed using Scanning Electron Microscopy (SEM) for imaging the surface topography of the heated areas. Energy dispersive x-ray spectroscopy (EDS) is performed to check for evidence of any chemical reaction. Focused Ion Beam (FIB) techniques are used to examine cross-sections of heated spots, both laterally and vertically. The first appearance of beadlike features several μm in depth is attributed to melting due to the textural similarities observed with the samples heated at one atmosphere. The melting temperature is determined by averaging the highest temperature without appearance of any bead (solid) and the lowest temperature with appearance of a bead (liquid).

Using the flash heating method, the melting of rhenium (Re) was measured to 47.4 GPa and 4600 K, a 5-fold extension of previous data (Fig. 64). Flash heating was successfully used in reproducing the previous melting curve of Mo measured by different techniques in the LHDAC, up to 45 GPa.

The difficulty in measuring melting temperatures of refractory metals in the LHDAC is perhaps best demonstrated by the discrepancy in the reported measurements on Ta. Using various methods to detect melting and measure temperatures, large differences in the melting slopes have been observed above 50 GPa, the chemical reactivity of Ta being the main difficulty. Flash heating measurements have now been successfully performed on Ta up to 85 GPa and 4318 K. Instead of heating the same sample at different locations at different temperatures, a given Ta sample was heated only at a single spot a single time at a predetermined temperature and pressure and then recovered to ambient conditions for further SEM, EDS and FIB processing and analysis (Fig. 65).

Heating at sub-liquidus temperatures only alters the surface to sub-micrometer levels, whereas melting produces significant structural changes several μm below the surface and a complete restructuring of the surface. EDS performed on Ta samples showed no sign of chemical reaction. The melting curve thus constructed explicity disagree with previous experimental reports.
Figure 66. Optical emission spectroscopy setup for plasma diagnostics during single crystal diamond growth. The inset photograph shows plasma and substrate inside the MPCVD deposition chamber. The local plasma-substrate environment, that is, plasma gas phase concentrations of activated species at the plasma boundary layer near the substrate surface. The underlying mechanisms controlling the size, position, and properties of the plasma discharge, particularly at the boundary layer near the substrate that affect diamond growth rate, are still not well understood. To investigate these processes, a non-intrusive diagnostic, such as optical emission spectroscopy (OES) has been developed at Carnegie. OES is a simple, in situ method that does not perturb the highly reactive plasma and probes electronically excited atoms and molecules, species concentrations, atomic relative densities, gas temperature, and the electron temperature of plasma discharge.

The emission intensity signal was collected using a fiber optic cable across a line of sight passing through the window of the observation port and pointed to the discharge inside the deposition chamber 15 cm away and 90° to the axis of the reactor (Fig. 66). A computer connected to the spectrometer was used for data acquisition with typical collection time of 100 ms.

Argon was added into the plasma in order to investigate the emission behavior of the plasma and its influence on the CVD diamond growth rate. Ar was selected due to its inertness, which does not perturb the plasma. Ar is excited to its radiative excited states mainly by a direct electron impact process. The radiative states of Ar have excitation thresholds close to that of the H atom in the n = 3 level.54

Visual observation showed that the luminous intensity of the plasma discharge increases as Ar is injected into the process chamber. The measured intensities of the three Ar lines also increase by adding argon into the deposition process chamber. However, the Hα, Hβ, and Hγ emissions stay constant. This suggests that Ar has little influence on the H chemistry and the contribution of argon to the excitation of H (n = 3) is negligible. Hence, Ar can be used as an actinometer, allowing the estimation of the relative concentration of species in their ground states within the plasma discharge.54, 55

The flash heating method can be employed with minimal modification of a standard LHDAC setup. It allows chemically clean, reliable and reproducible measurements of melting curves of metals with error less than 200°.

Optical Emission Diagnostics of CVD Diamond Growth – A key aspect of single crystal diamond growth via microwave plasma assisted chemical vapor deposition (MPCVD) is in-process control of

Figure 67. Strain distribution in a 400 nm gold single crystal at 1.7 GPa, as detected by the recently developed coherent diffraction imaging technique. (a) Crystal shape and surface truncated (100) and (111) planes. (b) and (c), top and bottom views. (d) – (f), side views, rotated 120° along the surface normal direction. Color represents the lattice strain (phase shift) from $-\pi/4$ to $\pi/4$. 54
X-Ray Nanoimaging – At HPSynC, Wenge Yang and co-workers from Carnegie, the APS, and University College London have made a major breakthrough in measuring the structure of nanomaterials under pressure. For the first time, a way to get around the severe distortions produced by high-energy x-rays that are used to image structures has been developed. The technique will eventually lead to new nanomaterials created under pressure and a greater understanding of material deformation. By averaging the diffraction patterns of the same single crystal using different sample alignments and using an algorithm developed by a group at the London Centre for Nanotechnology, it is possible to compensate for distortion and improve spatial resolution by two orders of magnitude. The technique was used to study a 400 nm gold nanocrystal from about 800 MPa to 6.4 GPa (Fig. 67).

These measurements were carried out on Beamline 34-ID-C at the APS. At first, as expected, the edges of the crystal become sharp and strained, but disappear under further compression. The crystal develops a more rounded shape at the highest pressure, implying an unusual plastic-like flow. In fact, nanoscale gold particles are very useful materials as they are about 60% stiffer compared with other micron-sized particles and could prove pivotal for constructing improved molecular electrodes, nanoscale coatings, and other advanced engineering materials.

4.5 Technical Development at Academic Nodes

Shock Wave Spectroscopy – Over the past few years, the Dlott group at Illinois has developed a shock wave spectroscopy apparatus that uses a one-box laser to launch flyer plates.56, 57 An 8 GHz photon Doppler velocimeter (PDV) is used to monitor the launch, flight and impact of 0.7 mm diameter Al flyer plates with various sample materials. The current arrangement of the system standard is shown in Fig. 68. The apparatus can be interfaced with a variety of spectroscopic tools. Under conditions used in the apparatus, the flyers are launched by a shock from the glass substrate right under the metal foil, so the flyers see very little laser intensity. They do not melt or vaporize. By stretching the laser pulses using an external pulse stretcher, the group has shown that it is possible to find conditions that eliminate the effects of reverberating shocks. The tilt is minimal, <1 μm, so that it introduces a time dispersion of 1 ns or less.

New diagnostic capabilities are under development. High-speed thermal imaging is used to measure temperature profiles in shocked inhomogeneous materials. Also, a Raman system is under construction and a few preliminary measurements have been made. Currently CDAC graduate students Will Shaw and Will Bassett are interfacing a femtosecond IR laser that will be used for IR absorption spectroscopy of shocked materials and liquids. Also, a 1 ns, 32 channel optical pyrometer to study the temperature dynamics of shocked reactive materials is also under development. All these improvements will expand the range of materials and conditions under which shock compression may be explored.

Finally, new sample fabrication techniques suitable for the study of powders and liquids are under development. These involve producing large-area samples having arrays of wells of known

Figure 68. Schematic of laser flyer launch system with photonic Doppler velocimeter (PDV). M = mirror, BS = beam splitter, BE = beam expander, DO = diffractive optic, OBJ = objective lens.
thickness that can be filled with sample materials. For instance, a sample might consist of a 50 x 50 mm$^2$ glass square having 100 wells, each slightly larger than the flyer plate and 50 μm thick. This becomes tricky when the sample is a volatile liquid, and for this application microfluidic arrays have been developed. This technology will be used to study particulate media that mimic soils and sand or solid propellants, and liquid media such as aqueous solutions and liquid explosives.

Diamond Anvil Cell Calorimeter — Zack Geballe, a student in the Jeanloz group at UC-Berkeley, has been developing a calorimeter for DACs, building on past modeling of heat transport. In collaboration with LLNL (Rip Collins) and the EECS department at UC Berkeley, he is making high-frequency, high-dynamic-range electrical diagnostics in order to measure heat capacity at high pressures. Together with Andrew Townley (EECS), he is using a combination of waveform generators, op-amps, electrical filters and digitizers to send up to 1 A of current through thin metal samples pressed against the table of a diamond anvil (which acts as a heat sink), and measuring the first and third harmonics of voltage across a 4-point probe. The goal is to adapt the method to high pressures in order to study pre-melting, melting and partial melting phenomena using up to 100 MHz modulated Joule heating. Currently, the EECS group is designing a suitably buffered voltage source with high harmonic purity at high frequency. In particular, they are modeling all details of the experiment, combining heat flow models, analytical calculations and LTSpice, a powerful electrical engineering code that represents a new tool for high-pressure research. More broadly, once developed, high-frequency electronics adapted to the diamond cell geometry could be useful for a range of dynamic heating, electrical and/or magnetic experiments inside DACs.

5. MANAGEMENT AND OVERSIGHT

5.1 CDAC Organization and Staff

CDAC is managed at Carnegie by a small staff comprised of the Director, Coordinator, Administrative Assistant and two Research Scientist/Laboratory Managers and two Research Scientists (Fig. 69). Daily operations of the Center are carried out by the Director, Coordinator and Assistant, while CDAC laboratory facilities at Carnegie are supervised by the Laboratory Managers. Research Scientists spearhead specific projects of interest to the CDAC research program. In addition to oversight of CDAC facilities at Carnegie, the Laboratory Managers assist CDAC visitors with experiments and sample preparation, in addition to training summer undergraduate students as part of the Carnegie Summer Scholars Program.

Russell Hemley, CDAC Director, is also a Staff Scientist at 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
- 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
- Morgan Phillips Hoople — CDAC Administrative Assistant
- Maddury Somayazulu — Lab Manager/Research Scientist
- Muhtar Ahart — Lab Manager/Research Scientist
- Ivan Naumov — Research Scientist
- Chang-sheng Zha — Research Scientist

Postdoctoral fellows, predoctoral students and visitors at Carnegie supported by the Institution, other grants, or outside fellowships often work with the CDAC group as part of their
research program. Their contributions also include training CDAC students, undergraduate summer scholars, and visitors in high-pressure experimental techniques:

- **Kadek Hemawan** (CVD Diamond)
- **Caitlin Murphy** (Geophysics)
- **Todd Zapata** (Magnetic/Electronic Properties of Materials)

### 5.2 CDAC Oversight

CDAC Steering and Advisory Committees have been instrumental in providing input on the direction of the CDAC research program (Fig. 70). 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** (University of West Georgia)
- **Gilbert W. (Rip) Collins** (LLNL)
- **Dana Dattelbaum** (LANL)
- **Daniel Dolan** (SNL)
- **Jon H. Eggert** (LLNL)
- **Marcus Knudson** (SNL)
- **Nenad Velisavljevic** (LANL)

*Figure 69. CDAC affiliated personnel at Carnegie for 2013-2014.*
The Advisory Committee assists with long-term strategic planning 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)
- Dawn Flicker (Sandia)
- David Funk (LANL)
- Alan J. Hurd (LANL)
- Chi-chang Kao (SLAC)
- Christian Mailhiot (LLNL)
- Tom Mehlhorn (SNL)

Figure 70. 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.

We encourage members of both CDAC oversight committees to attend regular HPCAT meetings and invite them to attend all CDAC functions. Members of both committees are updated regularly on progress in the scientific program, innovations in technique development, and plans for outreach.
APPENDIX I: CDAC Publications and Presentations for 2013-2014

We list publications and presentations for 2013-2014, 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


Chen, B., K. L. C. N. An, W. Yang, V. V. Struzhkin, and H. K. Mao, Pressure tuning of Fermi surface topology of optimally doped BaFe121.6Ni0.1As2, Phys. Rev. B, submitted.


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 mantagite (La\textsubscript{0.75}Ca\textsubscript{0.25}MnO\textsubscript{3}) under pressure, *Phys. Rev. Lett.*, submitted.


Efthimiopoulos, I., A. Yaresko, V. Tsurkan, J. Diesen, A. Loidl, C. Park, and Y. Wang, Multiple pressure-induced transitions in HgCr\textsubscript{2}S\textsubscript{4}, *Appl. Phys. Lett.* **103**, 201908 (2013).


Gleason, A. E. and W. L. Mao, Strength of iron at core pressures and evidence for a weak Earth's inner core, Nature Geosci. 6, 571-574 (2013).


Jacobsen, M. K., Y. Meng, R. S. Kumar, and A. L. Cornelius, High pressure structural and transport measurements of InTe, GaTe, and InGaTe$_2$, J. Phys. Chem. Solids 74, 723-728 (2013).


Kumar, R. S., Y. Zhang, A. Thamizhavel, A. Svane, G. Vaitheeswaran, V. Kanchana, Y. Xiao, P. Chow, C. Chen, and Y. Zhao, Pressure induced valence change of Eu in EuFeAs$_2$ at low temperature and high pressures probed by resonant inelastic x-ray scattering Appl. Phys. Lett. 104, 042601 (2014).

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 control stoichiometry and properties, Crystal Growth Design 13, 303-307 (2013).
Lavina, B., P. Dera, and Y. Meng, Synthesis and microdiffraction at extreme pressures and temperatures, J. Vis. Exp. 80, e50613 (2013).


Liu, J., J. F. Lin, A. Alatas, and W. Bi, Sound velocities of bcc-Fe and Fe_{0.85}Si_{0.15} alloy at high pressure and temperature, *Phys. Earth Planet. Inter.* **233**, 24-32 (2014).


Rainey, E. S. G. and A. Kavner, Peak scaling method to measure temperatures to the laser-heated diamond anvil cell and application to the thermal conductivity of MgO, J. Geophys. Res., submitted.


Zeng, Z., N. Liu, Q. Zeng, Y. Ding, S. Qu, Y. Cui, and W. L. Mao, Elastic moduli of polycrystalline Li$_1$Si$_4$ produced in lithium ion batteries, *J. Power Sources* **242**, 732-735 (2013).


Zhang, L., Y. Meng, I. Kantor, and W. L. Mao, Experimental evidence for iron inrichment in (Mg,Fe)$_3$SiO$_3$ perovskite relative to perovskite, *Earth Planet. Sci. Lett.*, submitted.


Zhuravlev, K. K., A. Goncharov, S. N. Tkachev, P. Dera, and V. Prakapenka, Vibrational, elastic, and structural properties of cubic silicon carbide under pressure up to 75 GPa: Implicatin for a primary pressure scale, J. Appl. Phys. 113, 113503 (2013).


**B. CDAC Presentations**


Cahill, D. G., Thermal conductance of weak and strong interfaces (invited), *Heraeus Seminar on Thermal Transport at the Nanoscale* (Bad Honnef, Germany, April 7-10, 2013).


Cahill, D. G., Extremes of heat conduction in molecular materials (invited), *Thomas Young Center Highlight Seminar, Imperial College* (London, UK, October 10, 2013).

Cahill, D. G., Thermal conductance of weak and strong interfaces (invited), *CECAM Workshop on Heat Transfer at Small Scales* (Zaragoza, Spain, Octobe 14-16, 2013).

Cahill, D. G., Thermal conductance of weak and strong interfaces (invited), *Hughes Research Laboratory Colloquium* (Malibu, CA, October 28, 2013).


Cahill, D. G., Extremes of heat conduction in molecular materials (invited), *Chemical and Materials Science Seminar, University of Minnesota* (Minneapolis, MN, November 12, 2013).


Cahill, D. G., Extremes of heat conduction in molecular materials (invited), *Department of Materials Science and Engineering Seminar, University of Tennessee* (Knoxville, TN, November 15, 2013).

Cahill, D. G., Extremes of heat conduction in molecular materials (invited), *Department of Materials Science and Engineering Seminar, Georgia Tech* (Atlanta, GA, November 18, 2013).


Cahill, D. G., Extremes of heat conduction in molecular materials (invited), *Department of Chemical Engineering Seminar, Illinois Institute of Technology* (Chicago, IL, February 19, 2014).

Cahill, D. G., Extremes of heat conduction in molecular materials (invited), *International Thermal Conductivity Conference, Purdue University* (West Lafayette, IN, April 28-30, 2014).


Daviau, K., Preliminary work on the melting of SiC at high pressure, Stewardship Science Academic Programs Symposium (North Bethesda, MD, February 19-20, 2014).


Dlott, D. D., Ultrafast vibrational spectroscopy and energy flow in molecules (invited), CECAM Workshop on Nanophononics (Bremen, Germany, August, 2013).

Dlott, D. D., Vibrational energy transfer on surfaces and in liquids (invited), American Chemical Society National Meeting (Indianapolis, IN, September, 2013).


Dlott, D. D., Molecular dynamics of explosives (invited), Rochester Institute of Technology Department of Chemistry and Materials Science (Rochester, NY, October, 2013).

Dlott, D. D., SFG studies of buried electrochemical interfaces (invited), American Chemical Society National Meeting (Dallas, TX, March 28, 2014).


Dlott, D. D., Vibrational energy transfer on surfaces and in liquids, MIT Modern Optics and Spectroscopy Seminar (Cambridge, MA, April, 2014).


Fei, Y., High pressure petrology and the Martian mantle and core (invited), APS-SCCM & AIRAPT-24 Joint Conference (Seattle, WA, July 7-12, 2013).

Fei, Y., C. A. Murphy, Y. Shibazaki, and H. Huang, Thermal equation of state of iron: Constraint on the density deficit of Earth's core, Eos Trans. AGU Fall Meet., Suppl. 94 (2013).


Geballe, Z., Brillouin studies of a highly-stable glass, CaSiO3, from 0 to 44 GPa, Stewardship Science Academic Programs Symposium (North Bethesda, MD, February 19-20, 2014).

Geballe, Z., S. M. Arveson, S. Speziale, and R. Jeanloz, Sound speed of amorphous CaSiO3 from 0 to 42 GPa, Eos Trans. AGU Fall Meet., Suppl. 94 (2013).


Goncharov, A., High pressure chemistry (invited), APS-SCCM & AIRAPT-24 Joint Conference (Seattle, WA, July 7-12, 2013).


Hemley, R. J., Molecules under pressure (invited), Flygare Lecture (University of Illinois, Urbana IL, May 8, 2013).


Hohensee, G., Metal-diamond interface thermal conductance with nitrogen defects at high pressures by time-domain thermoreflectance, Stewardship Science Academic Programs Symposium (North Bethesda, MD, February 19-20, 2014).


Jugle, M., Deformation and transformation textures in the NaMgF₃ perovskite to post-perovskite system, Stewardship Science Academic Programs Symposium (North Bethesda, MD, February 19-20, 2014).

Kaercher, P., Understanding lower mantle rheology from two-phase deformation experiments, Stewardship Science Academic Programs Symposium (North Bethesda, MD, February 19-20, 2014).


Lazaraz, J., Compression mechanism and equation of state of thaumasite up to 10 GPa, 2013 CDAC Annual Review (Argonne, IL, September 16, 2013).

Lee, K. K. M., Sinking deep in to a C-rich planet: Using experiments to constrain planetary interiors, YCAA Seminar, Yale University (New Haven, CT, February 18, 2014).


Lim, J., Origin of pressure-induced volume collapse in Dy, Tb, Gd, and destruction of dense kondo state in CeBa, to 120 GPa, Stewardship Science Academic Programs Symposium (North Bethesda, MD, February 19-20, 2014).


Marquardt, H. and L. Miyagi, Strength of (Mg,Fe)O ferropericlase in Earth’s lower mantle, Eos Trans. AGU Fall Meet., Suppl. 94 (2013).


Mauger, L., M. S. Lucas, J. A. Munoz, S. J. Tracy, and B. Fultz, Anharmonic phonon behavior in alpha-Fe at high temperatures, TMS 2013 Neutron and X-Ray Studies of Advanced Materials VI: Centennial and Beyond (San Antonio, TX, March 5, 2013).


McWilliams, R. S., Toward measurements of volatile behavior at realistic pressure and temperature conditions in planetary deep interiors, Eos Trans. AGU Fall Meet., Suppl. 94 (2013).


Miyagi, L., Deformation studies of lower mantle mineral phases and seismic anisotropy in the deep Earth (invited), Eos Trans. AGU Fall Meet., Suppl. 94 (2013).

Miyagi, L., H. Marquardt, and H. P. Liermann, Radial x-ray diffraction at the xtreme conditions beamline of PETRA III: In-situ texture analysis of a mixture of perovskite and ferropericlase to 1100 K and 40 GPa, Eos Trans. AGU Fall Meet., Suppl. 94 (2013).


Schilling, J. S., Pressure-induced electron localization/delocalization effects in alkali and rare earth metals (invited), *Institut für Festkörperphysik, Karlsruher Institut für Technologie* (Karlsruhe, Germany, June 13, 2013).


Schilling, J. S. and G. Schmiedeshoec, Dilatometry and high pressure experiments: Past, present, and future (invited), *Department of Physics Colloquium, Iowa State University* (Ames, IA, November 13, 2013).


Uhoya, W., High pressure effects on the superconductivity in rare earth doped CaFe2As2, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).


Zurek, E., Building a chemical intuition under pressure: Prediction of novel hydrides (invited), 6th CTTC Theoretical Chemistry Conference (Krakow, Poland September 2013).

Zurek, E., Building a chemical intuition under pressure: Prediction of alkali metal polyhydrides and subhydrides (invited), Joint APS-SCCM & AIRAPT 24 Conference (Seattle, WA, July 7-12, 2013).

Zurek, E., Building a chemical intuition under pressure: Prediction of alkali metal polyhydrides (invited), Condensed Matter Seminar, University of Toronto (Toronto, Canada, October, 2013).

Zurek, E., Structure prediction from first principles calculations (invited), MRSEC/CNFM Conference for Undergraduate Women in Physical Sciences - WoPhys (Lincoln, NE, October, 2013).
Zurek, E., Building a chemical intuition under pressure: Prediction of alkali metal polyhydrides and subhydrides (invited), *Department of Chemistry Seminar, SUNY Geneseo* (Geneseo, NY, October, 2013).


Zurek, E., Building a chemical intuition under pressure: Prediction of alkali metal polyhydrides and subhydrides (invited), *High Pressure Seminar, Max Planck Instutit fur Chemie* (Mainz, Germany, June 2013).


Zurek, E., Structure prediction from first principles (invited), *Texas Women’s University* (Dallas, TX, March, 2014).
APPENDIX II: CDAC Synchrotron Users/Experiments (APS and NSLS) for 2013-2014

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 in HPCAT obtained by CDAC, the support generated by SSAP funding made possible significant scientific productivity of the state-of-the-art high-pressure facility.

<table>
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<th>Dates</th>
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<tr>
<td>Z. Zhao</td>
<td>Stanford University</td>
<td>High pressure study of Sb₂O₃ and MoSe₂</td>
<td>May 30-June 1, 2013</td>
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<td>Z. Jenei</td>
<td>LLNL</td>
<td>Ultrasound study of Pr</td>
<td>May 31-June 4, 2013</td>
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<tr>
<td>J. Zhu</td>
<td>LANL</td>
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<td>June 1-3, 2013</td>
</tr>
<tr>
<td>L. Zhang</td>
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<td>Physical properties of silicates at high pressure</td>
<td>June 1-3, 2013</td>
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<tr>
<td>Y. Peng</td>
<td>HPsynC</td>
<td>IXS investigating TiM edge</td>
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<tr>
<td>Y. Ding</td>
<td>ANL</td>
<td>High-pressure IXS study of Fe M23 edge</td>
<td>June 1-6, 2013</td>
</tr>
<tr>
<td>C. Tracy, M. Lang &amp; A. Romanenko</td>
<td>University of Michigan GSI Darmstadt</td>
<td>The response of actinide oxides to irradiation fields of fission track energies</td>
<td>June 1-8, 2013</td>
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<tr>
<td>Y. Kono</td>
<td>HPCAT</td>
<td>Development of ultrasonic measurement of liquid</td>
<td>June 5-6, 2013</td>
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<tr>
<td>S. MacLeod</td>
<td>Atomic Weapons Establishment, UK</td>
<td>Melting of uranium</td>
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<td>H. Cynn</td>
<td>LLNL</td>
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<td>W. Yang</td>
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<td>High P-T study of SiSn liquid phase</td>
<td>June 6-9, 2013</td>
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<tr>
<td>M. Pravica, L. Bai, &amp; A. Romanenko</td>
<td>University of Nevada – Las Vegas</td>
<td>Studies of oxygen- and nitrogen-containing compounds subjected to extreme conditions using x-ray Raman spectroscopy</td>
<td>June 6-9, 2013</td>
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<tr>
<td>Q. Smith</td>
<td>University of Nevada – Las Vegas</td>
<td>X-ray induced decomposition</td>
<td>June 6-9, 2013</td>
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<tr>
<td>G. Guardala</td>
<td>University of Nevada – Las Vegas</td>
<td>High pressure studies of nitrogen-, oxygen-, and fluorine-containing compounds</td>
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<tr>
<td>Q. Hu</td>
<td>George Mason University</td>
<td>High pressure behaviors of coesite</td>
<td>June 8-10, 2013</td>
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<tr>
<td>X. Chen</td>
<td>Carnegie</td>
<td>TaS₂ diffraction under pressure</td>
<td>June 8-10, 2013</td>
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<tr>
<td>Y. Ye, S. H. Shim, Q. Zhang &amp; C. Nisr</td>
<td>Arizona State University</td>
<td>High pressure properties of mineral physics in subduction oceanic crust</td>
<td>June 8-11, 2013</td>
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<tr>
<td>Y. Peng</td>
<td>HPsynC</td>
<td>TiH₅ diffraction under high pressure and high temperature</td>
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<tr>
<td>S. Yu, E. J. Kim</td>
<td>Seoul National University, Korea</td>
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<td>Name</td>
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<td>C. Stan</td>
<td>Princeton University</td>
<td>(Mg,Fe)GeO$_2$ perovskite-postperovskite compression</td>
<td>June 12-14, 2013</td>
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<tr>
<td>T. Duffy &amp; G. Finkelstein</td>
<td>Princeton University</td>
<td>High pressure phase transition in YIG</td>
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<td>Y. Kono</td>
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<tr>
<td>R. Chellappa &amp; N. Velisavljevic</td>
<td>LANL</td>
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<tr>
<td>L. Bai</td>
<td>University of Nevada - Las Vegas</td>
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<td>B. Chen</td>
<td>University of Illinois - Urbana-Champaign</td>
<td>High-pressure single-crystal x-ray microdiffraction investigation of s-triazine derivatives</td>
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<tr>
<td>P. Dera</td>
<td>University of Chicago</td>
<td>High-pressure single-crystal x-ray microdiffraction investigation of s-triazine derivatives</td>
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<td>A. Connolly</td>
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<td>L. Zhang</td>
<td>Carnegie</td>
<td>Physical properties of silicates at high pressure</td>
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<td>J. Baker</td>
<td>University of Nevada - Las Vegas</td>
<td>High P-T thermo-electric measurements of Cu, Bi, and organics</td>
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<td>Structure and reactivity of high P-T water at mafic and ultramafic mineral surfaces</td>
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<td>Studies on CO-D$_2$O, Co-Zr-Nb metallic glass interaction with H$_2$</td>
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<td>S. Wang &amp; J. Liu</td>
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<td>C. McDonald &amp; P. Nasreen &amp; D. Antonio</td>
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<tr>
<td>Name</td>
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<td>Project Description</td>
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<td>B. Cochain</td>
<td>University of Edinburgh, UK</td>
<td>Effect of high pressure and temperature on the viscosity of molten fayalite and ferrosilite</td>
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<td>G. Guardala</td>
<td>University of Nevada – Las Vegas</td>
<td>Irradiation of perfluorocarbons</td>
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<td>Q. Smith</td>
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<td>Synchronizing synchrotron XRD with flash melting technique</td>
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B. U2A Infrared Beamline

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 provides partial salary support for Beamline Scientist Zhenxian Liu, as well as beamline upgrades and supplies.

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<td>S. Wang</td>
<td>Stanford University</td>
<td>Monitoring the bandgap of mixed valent CsAuI and CsAuBr$_3$ at high pressure</td>
<td>June 26-28, 2013</td>
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<tr>
<td>Z. Zhao</td>
<td>Stanford University</td>
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<td>S. Wang</td>
<td>Stanford University</td>
<td>High pressure infrared spectroscopic study on metallization of 3D topological insulators Ag$_2$Te and Ag$_2$Se</td>
<td>June 29-30, 2013</td>
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<tr>
<td>X. Xi</td>
<td>BNL</td>
<td>Evolution of superconductivity with pressure in iron-based superconductors studied by infrared spectroscopy</td>
<td>July 7-16, 2013</td>
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<tr>
<td>R. Liu</td>
<td>Jilin University</td>
<td>Pressure induced metal-insulator transition in VO$_2$ bulks and nanomaterials</td>
<td>July 17-25, 2013</td>
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<td>Q. Li</td>
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<tr>
<td>P. Bowden</td>
<td>LANL</td>
<td>High pressure chemistry of simple molecules: Hydrazine and its methylated derivatives</td>
<td>July 25-30, 2013</td>
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<td>N. Mack</td>
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<td>T. Yu</td>
<td>New Jersey Institute of Technology</td>
<td>High pressure IR and XRD studies of multiferroic orthorhombic REMnOs$_3$</td>
<td>July 31-August 2, 2013</td>
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<td>T. Wu</td>
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<td>T. Tyson</td>
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<tr>
<td>W. Du</td>
<td>State University of New York at Stony Brook</td>
<td>Investigation of water content of high pressure experiment recovered sample</td>
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<td>Z. Liu</td>
<td>Carnegie</td>
<td>Infrared study for dense hydrogen under wide simultaneous $P$-$T$ conditions</td>
<td>August 7-10, 2013</td>
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<tr>
<td>R. Chellappa</td>
<td>LANL</td>
<td>Role of mode anharmonicity in initiation of high explosives</td>
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<td>D. Dattelbaum</td>
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<tr>
<td>M. Bishop</td>
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<td>High $P$-$T$ phase stability and decomposition boundary investigation of FOX 7</td>
<td>August 21-25, 2013</td>
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<td>N. Velisavljevic</td>
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<tr>
<td>H. Feng</td>
<td>Montclair State University</td>
<td>Chemical study of mental chelation on functionalized graphene surface for development of metal catalysis and sensors</td>
<td>September 12-13, 2013</td>
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<td>Z. Liu</td>
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<tr>
<td>X. Xi</td>
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<td>J. Musfeldt</td>
<td>University of Tennessee</td>
<td>Pressure-induced in the magnetoelastic coupling of Co(dca)_2 by synchrotron infrared spectroscopy</td>
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<td>B. Chen L. Kong</td>
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<td>High pressure IR and XRD study of mix-stacking Nano-ZnS</td>
<td>October 26-28, 2013</td>
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<td>B. Chen L. Kong</td>
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<td>X. Xi</td>
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<tr>
<td>H. Feng</td>
<td>Montclair State University</td>
<td>Chemical study of mental chelation on functionalized graphene surface for development of metal catalysis and sensors</td>
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<tr>
<td>D. Reaman</td>
<td>Army Research Laboratory</td>
<td>High pressure IR analysis of compressed gas mixtures with application to high-energy and super-hard materials</td>
<td>February 12-14, 2014</td>
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<tr>
<td>X. Xi</td>
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<td>H. Zheng K. Li</td>
<td>HPSTAR</td>
<td>The reaction mechanism and dynamics of acetonitrile under high pressure</td>
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<td>J. Zhu L.S. Zhang</td>
<td>LANL Chinese Academy of Sciences</td>
<td>Anomalous antiferromagnetic metallic evolution of CaCrO_3 single crystal under high pressure: an IR spectroscopy study</td>
<td>February 22-March 1, 2014</td>
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<tr>
<td>J. Tse J. Zhao</td>
<td>University of Saskatchewan</td>
<td>Pressure induced magnetic and insulator to nano-organometallic radical complexes</td>
<td>Mar. 6-8, 2014, Mar. 9, 2014</td>
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<tr>
<td>D. Reaman</td>
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<td>A. Plonka</td>
<td>State University of New York at Stony Brook</td>
<td>Pressure induced polymerization of dyines in assembled ococrystals</td>
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<td>Z. Liu X. Xi</td>
<td>Carnegie BNL</td>
<td>Infrared spectroscopy of H_2O up to 100 GPa</td>
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<td>L. Kong G. Liu</td>
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<td>High pressure IR and XRD study of mix-stacking nano-ZnS</td>
<td>Mar. 28-30, Mar. 31-Apr. 1, 2014</td>
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<td>Z. Liu Y. Ma Y. Lee</td>
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<td>Pressure-induced trapping of large cations and molecules in small-pore zeolites</td>
<td>Apr. 1-2, 2014</td>
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<td>C. Ma B. Yang J. Chen H. Zhu Q. Cui</td>
<td>HPSTAR Jilin University</td>
<td>High pressure infrared spectroscopy studies of cyclopentane</td>
<td>Apr. 3-5, 2014 Apr. 6, 2014</td>
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<td>A. Campbell B. Chidester E. Tompson R. Fisher</td>
<td>University of Chicago</td>
<td>High pressure optical absorption across an electronic spin transition in (Mg,Mn)O</td>
<td>Apr. 7-9, 2014</td>
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<td>A. Campbell B. Chidester E. Tompson R. Fisher</td>
<td>University of Chicago</td>
<td>Spectroscopic properties of pyrite (FeS2) at high pressure</td>
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<td>R. Liu Q. Li</td>
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<td>Apr. 16-18, 2013</td>
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<td>Z. Liu X. Xi</td>
<td>Carnegie BNL</td>
<td>Infrared spectroscopy of H2O up to 100 GPa</td>
<td>Apr. 19-22, 2014</td>
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<td>M. Sangwan</td>
<td>Carnegie</td>
<td>Kinetic study of methanol synthesis from carbon dioxide and hydrogen at elevated temperature and pressures</td>
<td>Apr. 24-25, 2014</td>
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<td>R. Chellappa M. Bishop N. Velisavljevic</td>
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