1. COVER PAGE

Federal Agency and Organization Element to Which Report is Submitted:
Department of Energy, National Nuclear Security Administration

Federal Grant Number Assigned by Agency: DE-NA0002006

Project Title:
Carnegie-DOE Alliance Center: A Center of Excellence for High Pressure Science and Technology

PI Name: Dr. Russell J. Hemley

Submission Date: February 28, 2016

DUNS Number: 0726417070000

Recipient Organization: Carnegie Institution of Washington
1530 P Street, NW
Washington, DC 20005

Grant Period: March 1, 2013 – February 28, 2018

Reporting Period: March 1, 2014 – February 28, 2015

Report Frequency: Annual

2. ACCOMPLISHMENTS

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, 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.[2]

Figure 1. *2014-2015 CDAC Partners.*

The mission of CDAC, which remains the same as it was at the inception of the Center, is to expand our understanding of materials behavior at extreme pressure-temperature (*P-T*) conditions, develop new facilities and methods to advance high *P-T* materials science, and support 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 maintains an integrated program of education, research and technical development to support the fundamental science that underlies the NNSA mission in stockpile stewardship and its legacy in national security.[3]

Box 1. CDAC Academic Partners for 2014-2015

- **David Cahill** (University of Illinois)
- **Przemek Dera** (University of Hawai'i)
- **Dana Dlott** (University of Illinois)
- **Brent Fultz** (California Institute of Technology)
- **Steven Jacobsen** (Northwestern University)
- **Raymond Jeanloz** (University of California – Berkeley)
- **Abby Kavner** (University of California – Los Angeles)
- **Kanani Lee** (Yale University)
- **Lowell Miyagi** (University of Utah)
- **James Schilling** (Washington University in St. Louis)
- **Yogesh Vohra** (University of Alabama – Birmingham)
- **Hans-Rudolf Wenk** (University of California – Berkeley)
- **Choong-shik Yoo** (Washington State University)
- **Eva Zurek** (SUNY – University at Buffalo)

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 headquartered at the Carnegie Institution of Washington and managed by **Russell J. Hemley** (Director), **Stephen A. 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 offsite facilities. Also at Carnegie, **Kadek Hemawan** supports efforts in CVD diamond growth, and **Ivan Naumov** provides expertise in computational theory.

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 country. 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.

In the following sections, we outline highlights from Year 2 of the current grant period (Year 12 of the Center's program).

2.1 SCIENTIFIC PROGRESS

Spectroscopic Steps to Stronger Steel – As iron is heated, the arrangement of the atoms in the solid changes several times before the iron finally melts. This unusual behavior is one reason why steel is so strong. The atomic-level details of how and why iron takes on so many different forms during heating remains a mystery, however. Recent work by Caltech CDAC Partner **Brent Fultz**, current and former Caltech CDAC students **Lisa Mauger**, **Matthew Lucas**, and **Jorge Muñoz**; and HPCAT Beamline Scientists **Yuming Xiao** and **Paul Chow** provides evidence for how iron's magnetism plays a role in the melting behavior of iron, and it is this detailed understanding that could help metallurgists develop better and stronger steel.

The laws of thermodynamics govern the natural behavior of matter, such as the temperature at which materials melt and freeze, and the preferred direction of chemical reactions. These same principles also determine the most stable arrangements of atoms in solids; in the case of iron, the stable arrangement changes several times with increasing temperature. From the room temperature, body-centered cubic (bcc) structure, iron adopts the face-centered cubic (fcc) structure at 912 °C (Fig. 1), and then becomes body-centered again at 1,394 °C, with a larger interatomic spacing, before and ultimately melting at 1,538 °C.

Iron is magnetic at room temperature, and previous work predicted that iron's magnetism favors the bcc phase at low temperatures. At 770 °C, however, iron loses its magnetism, but maintains its open, bcc structure well beyond this magnetic transition, suggesting that another effect must be responsible for the unusual sequence of crystal structure preference for iron at high temperatures.

Using nuclear resonant inelastic x-ray scattering (NRIXS) spectroscopy at HPCAT, Mauger and co-workers investigated the vibrational properties of iron with increasing temperature. The vibrational properties of materials are closely tied to temperature, and coupling these vibrational measurements with previously known data about the magnetic behavior of iron at high temperatures led to the conclusion that the vibrational entropy of iron is much larger than originally suspected. In fact, the excess vibrational entropy is similar to the entropy contribution from magnetism, suggesting that magnetism and atomic vibrations interact synergistically at moderate temperatures. This excess entropy increases the stability of the bcc structure even as the sample is heated past the magnetic transition. The NRIXS technique allowed the group to obtain the first experimental evidence that magnons (magnetic excitations) and phonons (vibrational excitations) interact to increase the stability of the bcc phase of iron at high temperatures.[4]

Because the NRIXS measurements were consistent with the theoretical calculations that were simultaneously carried out by collaborators in the laboratory of Jörg Neugebauer at the Max-Planck-Institut für Eisenforschung (Iron Research), Fultz and Mauger also contributed to the validation of a new computational model. With a better computational model for the thermodynamics of iron at different temperatures—one that takes into account the effects of both magnetism and atomic vibrations—metallurgists will now be able to more accurately predict the thermodynamic properties of iron alloys as they alter their formulations.[5]

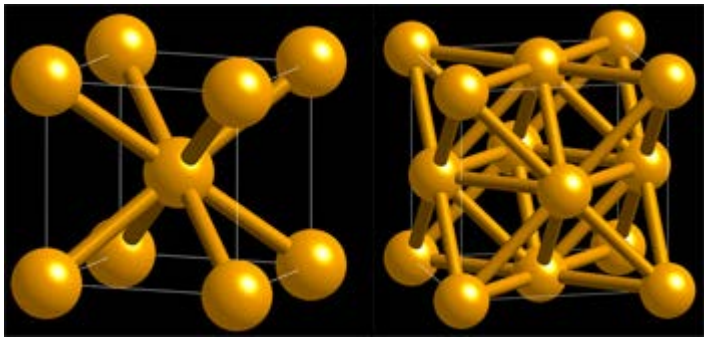

Figure 2. *Crystal structures of iron. Left: body-centered cubic (bcc); right: face-centered cubic (fcc).*

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 terapascal range (TPa, tens of millions of atmospheres). The possible existence of carbon-rich planets has created interest in the behavior of carbon at these conditions. Now, 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), has carried out ramp compression experiments on carbon to 5 TPa at the National Ignition Facility (NIF) on the Livermore Laboratory site.

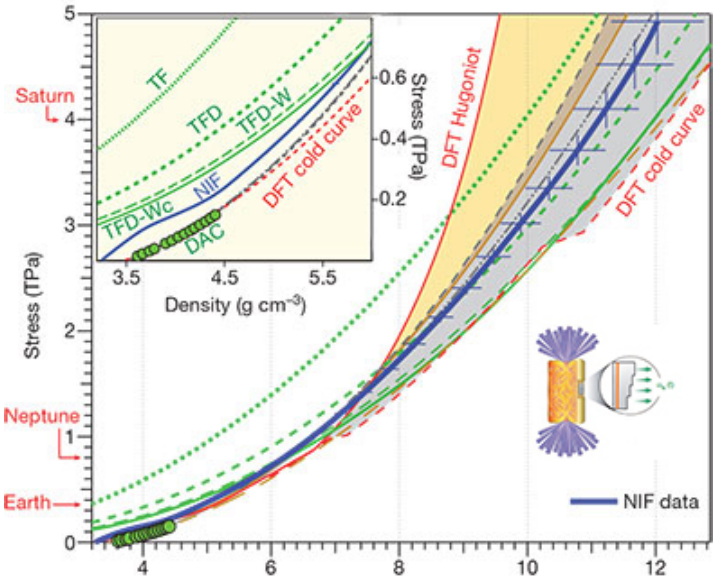

Figure 3. *Stress versus density for carbon. Current NIF data are shown in blue, with error bars of 1σ. The shaded region defines the approximate limits of uncertainty in the equation of state. Static diamond anvil cell data are shown as green circles. Various theoretical models (green and red lines) and fits to static data (grey lines) are shown for comparison.* ***Inset:*** *6mm diameter, 11 mm high gold-coated hohlraum containing the synthetic diamond target.*

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 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. 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 (Fig. 1).

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.[6]

Carbon in the Core – Seismic shear waves passing through the Earth's core travel at about half the speed of iron and related alloys at similar pressures, consistent with a "density deficit" in the core relative to iron or iron-nickel alloys. It is now widely accepted that, in addition to an iron-nickel alloy, Earth's inner core contains one or more lighter elements. The identity of these lighter elements, however, has been the subject of much debate for several decades. Among the candidate elements most likely to account for the density deficit are sulfur, carbon, silicon, oxygen or hydrogen. Alternatively, "softened" shear wave velocities at core pressures have been attributed to the presence of liquid, which calls into question the solid nature of the inner core.

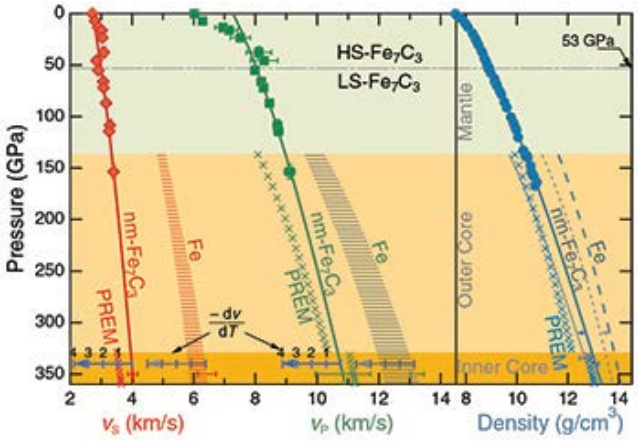

Figure 4. *Shear (red) and compressional (green) sound velocities and density (blue) of Fe7C3 with pressure. Solid lines represent fits to the data from a third-order Birch Murnaghan equation of state. Shaded areas (red, green) and the long-dashed blue line show extrapolations for pure hpc-Fe from a range of different measurements. PREM: Preliminary Earth Reference Model.*[1]

Using nuclear resonant inelastic scattering (NRIXS) spectroscopy to determine the phonon density of states of the model iron alloy Fe_7C_3, CDAC graduate student **Bin Chen** and co-workers from the University of Illinois, HPCAT, and the X-ray Science Division at the Advanced Photon Source (APS), were able to determine the shear wave velocities of the material at high pressures and extrapolate the results to the pressure of the inner core. The measurements, carried out at Sector 3 of the APS, suggest that Fe_7C_3 provides a good match for the inner core, without the need to consider partial melting or large temperature effects (Fig. Chen 1). Syncrotron Mossbauer Spectroscopy (Sector 3) and x-ray emission spectroscopy Sector 16, HPCAT) carried out on the same samples provided information on the nature of the magnetic and electronic spin transitions with pressure, confirming the low-spin character of Fe at the pressure of the inner core.

The proposal the inner core has the composition Fe_7C_3 has dramatic implications for the amount of carbon stored within the Earth. Current models suggest that the Earth's interior is depleted in carbon, but an inner core with the proposed composition would imply that up to two-thirds of Earth's carbon is stored within the core.[7]

Super TNT? – In a paper recently released in *Physical Review Letters*, a group including CDAC graduate student **Dane Tomasino**, CDAC Partner **Choong-shik Yoo** (both from Washington State University), and **Jesse Smith** from HPCAT, report the significant discovery of a novel layered, singly-bonded polymeric form of nitrogen (LP-N). The material is synthesized by laser-heating nitrogen at pressures between 125-180 GPa. This

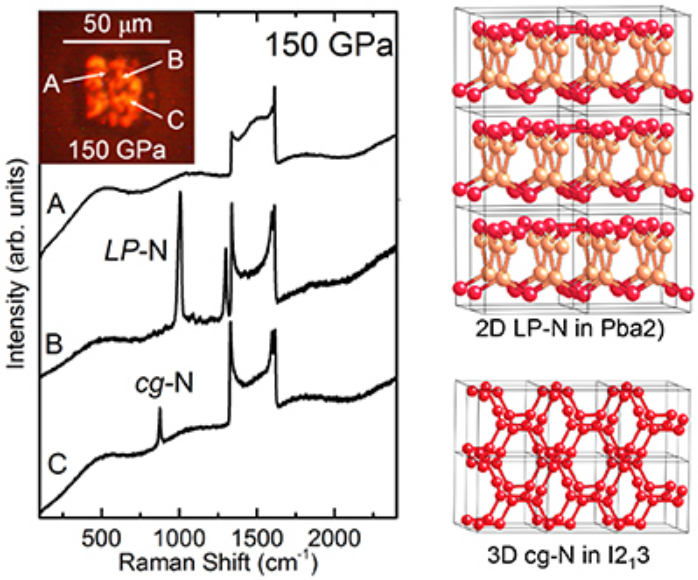

Figure 5. *Left: Raman spectra of laser-heated nitrogen at 150 GPa and ambient temperature, obtained in the three distinctive regions in the inset. (A) black amorphous, (B) new LP-N, and (C) gn-N. LP-N shows two characteristic peaks with exceptionally strong intensities. Right: Crystal structures of 2D LB-N in (Pba2) and 3D cg-N in I213. LP-N consists of two distinctive nitrogen sites, which gives rise to two characteristic Raman bands.*

new material exhibits a wide range of novel properties, including a colossal Raman cross section, at this point the largest of all known solids. Other properties include extremely high density (ρ=4.0 g/cm^3), even compared to diamond (3.5 g/cm^3), a large stiffness (K_o=345 GPa) rivaling superhard cubic-BN, and a potentially high energy density exceeding its sister phase cg-N and five times that of TNT. Only a few solids can have all these properties together. This places LP-N in the class of materials such as diamond and graphene, which can potentially lead to materials innovations in the future.

Importantly, the studies of LP-N also provide a new constraint on the nitrogen phase diagram, highlighting an unusual symmetry lowering 3D cg-N -> 2D LP-N transition with pressure, in contrast to more commonly found 2D to 3D transitions such as the graphite -> diamond. The transition from cg-N to LP-N points to an enhanced electrostatic contribution to the stabilization of the densely packed layer structure of LP-N.[8]

Growing Complexity in the Simplest Element – Studies of molecular hydrogen at static or sustained multimegabar pressures are difficult as a result of challenges in containing the samples under these conditions, and making accurate measurements of the material sample in the diamond anvil cell. Nevertheless, recent advances in diamond anvil cell techniques have now enabled measurements on hydrogen to above 300 GPa at room temperature, and new findings are providing additional evidence for the complexity of this enigmatic element.

In recent work at Carnegie, Raman measurements of hydrogen and deuterium have been carried out to new regimes of pressure and temperature - to 325 GPa at 300 K. CDAC Research Scientist **Chang-sheng Zha** and CDAC Director **Russell Hemley**, together with Carnegie's **Ronald E. Cohen** and **Ho-kwang Mao**, conducted the research. The 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 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.

Although it would appear to be the simplest element in the periodic table, hydrogen continues to reveal surprising behavior that differs from that expected from long held

views. 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.[9]

Turning Hydrogen into "Graphene" – New work from Carnegie's **Ivan Naumov** and **Russell Hemley** delves into the chemistry underlying some surprising recent observations about hydrogen and reveals remarkable parallels between hydrogen and graphene under extreme pressures. Their work is the cover story in the December issue of *Accounts of Chemical Research*.

Hydrogen is the most abundant element in the cosmos. With only a single electron per atom, it is deceptively simple. As a result, hydrogen has been a testing ground for theories of the chemical bond since the birth of quantum mechanics a century ago. Understanding the nature of chemical bonding in extreme environments is crucial for expanding our understanding of matter over the broad range of conditions found in the universe.

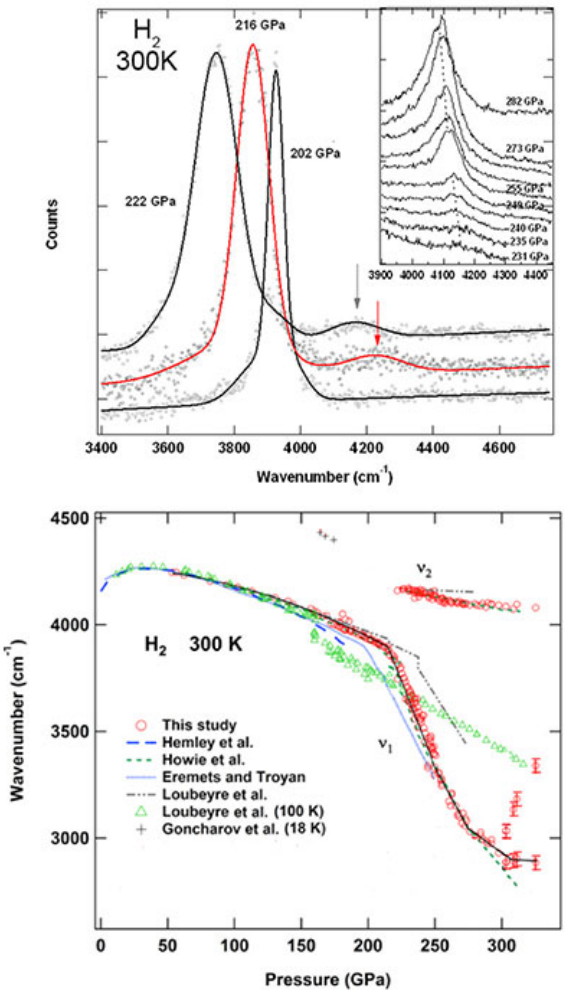

Figure 6. *Top: Hydrogen vibron spectra across the I-III-IV transition. Bottom: Pressure dependence of Raman vibrons at 300 K*

Observing hydrogen's behavior under very high pressures has been a great challenge for researchers. But recently teams have been able to observe that at pressures of 2-to-3.5 million times normal atmospheric pressure it transforms into an unexpected structure consisting of layered sheets, rather than a close-packed metal as had been predicted many years ago. These hydrogen sheets resemble the carbon compound graphene. Graphene's layers are each constructed of a honeycomb structure made of six-atom carbon rings. This conventional "carbon graphene" has unusual electronic properties that are revolutionizing advanced technology.

The new work from Naumov and Hemley shows that the stability of the unusual hydrogen structure arises from the intrinsic stability of its hydrogen rings. These rings form because of aromaticity which is well understood in carbon containing-molecules such as benzene, as well as in graphene. In each of these aromatic structures, electrons delocalize through the ring to increase stability. Naumov and Hemley's study indicates that hydrogen becomes a dark, poorly conducting metal like graphite instead of a conventional shiny metal and a good conductor, as was originally predicted over many decades of study.

Though the discovery of the graphene character of dense hydrogen has come as a surprise to many, chemists thirty years ago – before the discovery of graphene – predicted the structure based on simple chemical considerations. Their work is validated and extended by new findings. The group's results indicate that chemical bonding occurs over a much broader range of conditions than people had previously considered. However, the structural

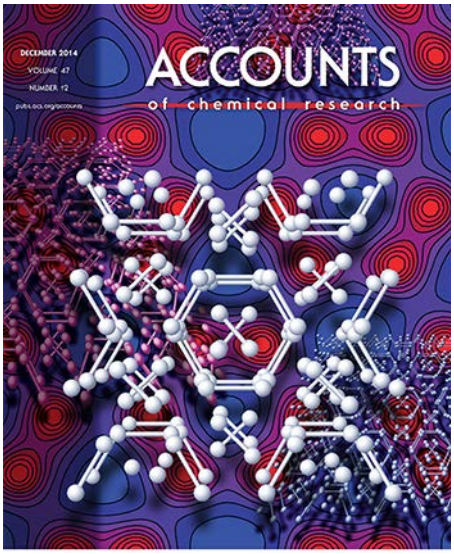

Figure 7. *Compressed hydrogen is inclined to adopt layered structures composed of distorted graphene-like layers. This tendency is driven by the aromatic and closed shell effect.*

effects of that chemical bonding under conditions can be very different than that observed under the ordinary conditions that are familiar to us.[10]

Hydrogen, Trapped – Understanding the basic chemical interactions in clathrate compounds is important in areas as diverse as energy storage and pharmaceutical development.

At **Carnegie**, **Timothy Strobel** and **CDAC** intern **Viktor Rozsa** (**Hillsdale College**, now at **University of Chicago**) have recently discovered extremely novel behavior in hydrogen-loaded hydroquinone (ß-HQ-H_2) clathrate under pressure. While the vast majority of materials contract under hydrostatic compression, the volume of ß-HQ-H_2 clathrate actually expands nearly 1% when compressed between 2.5 and 3.0 GPa. Over this pressure range, the negative bulk modulus and negative linear compressibility along two crystallographic axes are a consequence of a change in hydrogen occupancy from one to three molecules in the structure.

The ß phase of hydroquinone (HQ), or quinol (1,4-benzenediol), has a clathrate structure that is capable of trapping small molecules less than ~4 Å in diameter. Clathrate cavities in ß-HQ clathrate cavities consist of six HQ molecules with $[OH]_6$ rings terminating the top and bottom of the cage along the *c* axis and benzene rings comprising the cage equator in the *a*-*b* plane. With increasing pressure under hydrogen loading, the characteristic hydrogen vibron increases discontinuously in frequency at around 1.4 GPa, concomitant with a more repulsive local environment for H_2.[11]

Dehydration Melting in the Deep – The high water storage capacity of minerals in Earth's mantle transition zone (410- to 660-kilometer depth) implies the possibility of a deep H_2O reservoir, which could cause dehydration melting of vertically flowing mantle. In recent work, CDAC Partner **Steve Jacobsen** (Northwestern), Carnegie-CDAC Research Scientist **Zhenxian Liu** (NSLS) and colleagues from the University of New Mexico, University of Southern California, and University of Wyoming have 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 examined 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

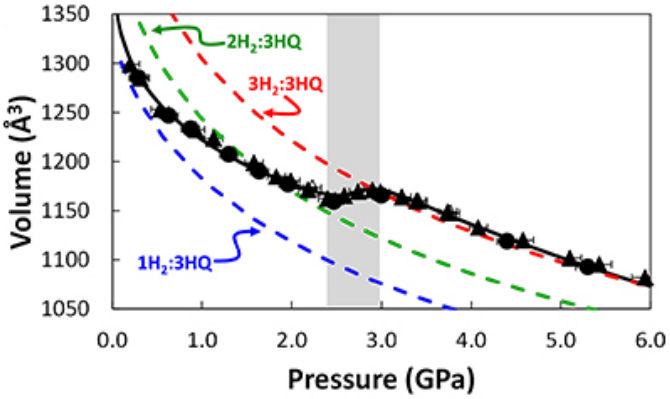

Figure 8. *Experimental unit cell volume as a function of pressure (points) compared with hypothetical assemblages of HQ and H_2 from the pure component equation of state (dashed lines). The shaded region between 2.4 and 3 GPa indicates where the unit cell volume increases with pressure.*

region of the transition zone and that dehydration melting may act to trap H_2O in the transition zone.[12] Their research was also featured in an article in *USA Today*.[13]

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.

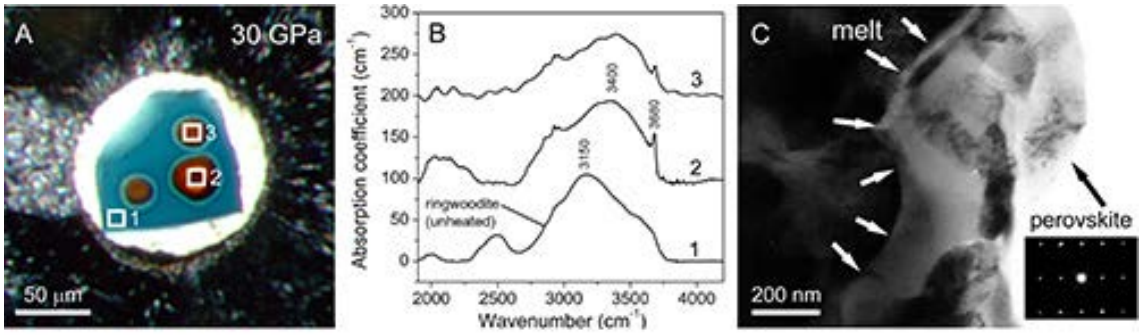

Figure 9. *(A) Single-crystal of hydrous ringwoodite (blue crystal) containing 1 wt % H2O inside a diamond-anvil cell at 30 GPa. The sample was laser heated to 1600°C in several spots (orange circles) to perform direct transformation to perovskite and (Mg,Fe)O. (B) Synchrotron-FTIR spectra of the recovered sample were collected with a 10 mm by 10 mm aperture at beamline U2A of the NSLS. Spectrum 1 is an unheated spot, characteristic of hydrous ringwoodite. Spectra 2 and 3 from within the laser heated spots exhibit modified IR-absorption spectra in the OH region, with a broad and asymmetric band at 3400 cm-1 (characteristic of OH in quenched glass) and a sharp peak (3680 cm-1) associated with brucite. On conversion to perovskite plus (Mg,Fe)O, dehydration melting occurred as intergranular melt, viewed by TEM in panel C. In this study, dehydration melting was detected just beneath the mantle transition zone from P-to-S converted phases using seismic data from NSF-Earthscope, US-Array.*

CDAC Graduate Student **Spencer Smith**, along with CDAC Academic Partner **Yogesh Vohra** and colleagues from the University of Alabama - Birmingham, used diamond anvil cell technology, Raman spectroscopy, synchrotron x-ray diffraction, and multiple *ab initio* harmonic frequency calculations to explore the solid-state transition behavior of Paracetamol (Figure 2, a commonly used analgesic and anti-pyretic) at hydrostatic pressures up to 21 GPa.

Figure 10. *Chemical structure of paracetamol ($C_8H_9NO_2$).*

Spectral measurements provide further evidence for a highly kinetically driven Form I --> 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.[14]

Novel Carbon Bonding at High Pressure **--** Only a small fraction of our planet's total carbon budget is found at the surface. In fact, Earth's mantle is thought to be the largest carbon reservoir. Carbonates, and in particular ferromagnesite ($(Mg,Fe)CO_3$), are likely candidates for deep-Earth carbon storage and therefore play a key role in the deep carbon cycle. The behavior of these carbonates at the high pressure and temperature conditions of Earth's interior is therefore of great interest for understanding global carbon cycling and storage.

A new paper, appearing in an upcoming issue of *Nature Communications*, reports unequivocal experimental evidence for tetrahedrally coordinated carbon in high pressure carbonates, obtained by combined experimental and theoretical studies carried out by a

group including former CDAC Student and Partner **Wendy Mao** (Stanford University) and CDAC Scientist **Zhenxian Liu** (NSLS).

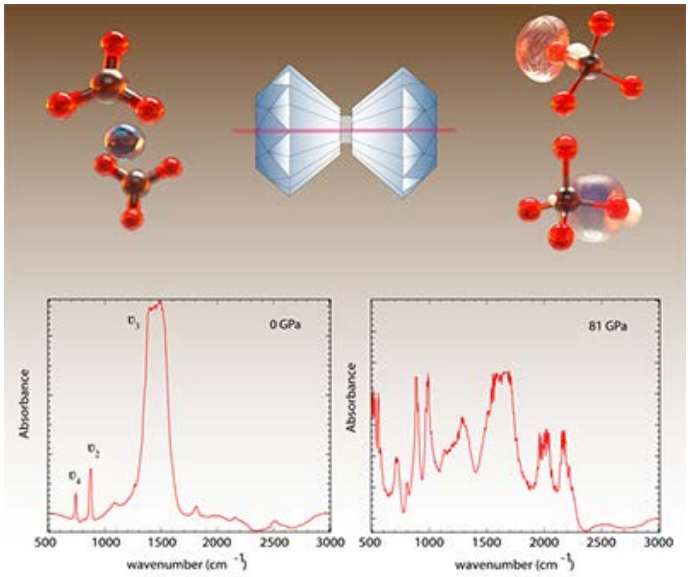

Figure 11. *Carbon environment and associated in situ infrared spectra of ferromagnesite at ambient conditions (left) and at high pressure (right). At ambient conditions, carbon exists as the carbonate ion, CO_3^{2-}. At high pressure, carbon adopts tetrahedral coordination as CO_4^{4-}.*

With the combination of *in situ* synchrotron infrared spectroscopic measurements carried out at high pressure, and *ab initio* calculations on the ferromagnesite structure, it was possible to identify a unique vibrational signature present only in the high-pressure phase, and thus a new carbon-oxygen bond forms in ferromagnesite under pressure. The new vibrational signature is assigned to tetrahedrally coordinated carbon atoms with asymmetric C-O bonds.

Ferromagnesite represents an important rock-forming mineral, fundamentally distinct from silicates in Earth's crust. At low pressure, carbon bonds to three oxygen atoms, while silicon bonds to four. Tetrahedrally coordinated carbonates likely exhibit dramatically different behavior compared to three-fold coordinated carbonates, including altered reactivity with other mantle phases and changes in chemical melt properties. This bonding behavior could therefore have significant implications for carbon reservoirs and fluxes, as well as for our understanding of the global geodynamic carbon cycle.[15]

Fullerene-Graphene Composite Material – Carbon exists in a variety of structural motifs as a result of its ability to adopt sp-, sp^2-, and sp^3-type bonding modes. Graphite, diamond, and lonsdaleite (hexagonal diamond) are well-established allotropic forms of carbon, but in recent years fullerenes, nanotubes, graphene and even amorphous carbon have received a increasing attention as a result of their unusual, and potentially technologically useful properties.

Glass-like carbon (GC) is a class of nongraphitizing carbon made by firing polymeric precursors such as phenolic resin or furfuryl alcohol resin in an inert atmosphere. Type I GC, which is produced at low temperatures, consists mainly of randomly distributed, curved graphene layer fragments. Type II GC, fabricated at high temperatures, contains self-assembled, fullerene-like, nanometer-sized spheroids dispersed within, and interconnected by, a three-dimensional disordered multilayer graphene matrix. Type II GC can therefore be envisaged as fullerene-like spheroids encased in disordered graphene layers with a nanostructure like that shown in Fig. 1, which has a number of similarities to mechanical metamaterials, but with statistical characteristic building blocks (that is, fullerene-like spheroids) at nanometre scales. It is well known that graphene has very high in-plane strength, while fullerene has a large volume deformation capacity, and so the hybrid type-II GC is expected to have the integrated features of both materials to possess exceptional mechanical properties.

At HPCAT, a group including Director **Guoyin Shen** and postdoctoral associate **Zhisheng Zhao**, along with collaborators from HPCAT, University of Chicago, Yanshan University and China University of Geosciences has found that the hybrid Type II

GC possesses a number of advantageous properties such as high strength (> 3 times stainless steel), high volume compression, superelastic (rubber-like) recovery from large volume deformation (~40% volume reduction), high uniaxial strain (up to 6% strain compared with that of the shape memory alloy), and a pressure-induced variable (zero or even negative) Poisson's ratio. Recently developed, *in-situ* techniques for direct volume determination, acoustic wave velocity measurements, and x-ray diffraction at HPCAT, along with molecular dynamics simulations, were employed to explore the nature of the unusual and pressure-tunable, compression and elastic properties. Controlling the concentration, size and shape of fullerene-like spheroids with tailored topological connectivity to graphene layers is expected to yield exceptional and tunable mechanical properties, similar to mechanical metamaterials, with a potentially wide range of applications.

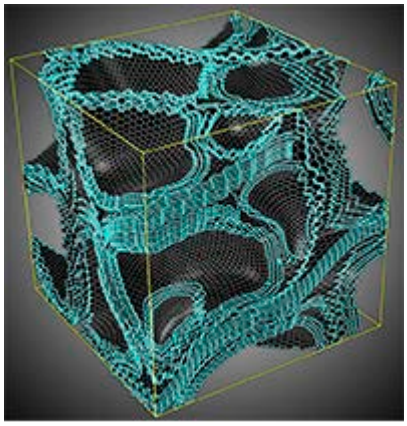

Figure 12. *Rendering of fullerene-like spheroids (black/grey) and matrix of graphene sheets (green). Spheroids are on the order of 5-10 nm in size.*

The discovery of fullerene-like spheroids encased in a disordered, multi-layer graphene matrix opens a route for the preparation of new forms of carbon that feature combinations of two or more carbon allotropes. Such combined forms may display properties superior to the properties of either of the components, and perhaps unique combinations of tailored mechanical and electronic properties may be obtained.[16]

2.2 TECHNIQUE DEVELOPMENT

Liquid-Liquid Transition in Cerium – The melting line of cerium metal is characterized by an unusual broad minimum at approximately 3.3 GPa. More recent work has extended the established pressure range of the melt line to nearly 30 GPa, where the melting temperature has risen to 1370 K from its minimum at 935 K. This behavior of the melting line suggests that two different liquid states exist on either side of 3.3 GPa. In fact, it has been conjectured since the 1970s that the nature of the isostructural volume collapse in the solid at 0.75 GPa, first discovered by Bridgman in 1927, is related to this phenomenon.

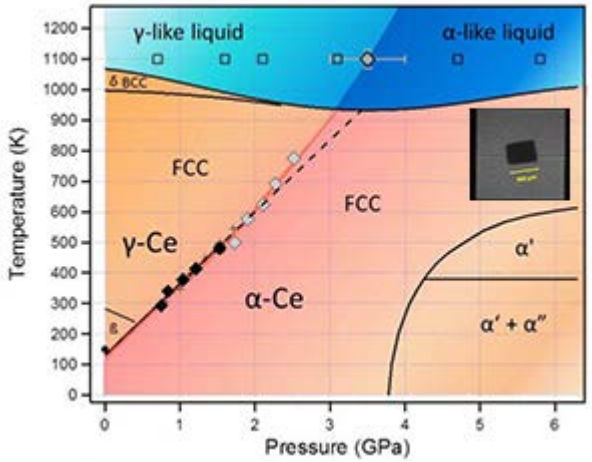

Figure 13. *Phase diagram for Ce metal showing the location of the minimum in the bulk modulus above the critical point (diamonds), and volume points from the radiography measurements. The gold diamond represents the inflection point in the P-V isotherm at 1100 K, at approximately 3.5 GPa.*

Using the large volume Paris-Edinburgh press at HPCAT Beamline 16-BM-B, **Yoshio Kono**, **Curtis Kenney-Benson**, and **Changyong Park** from HPCAT worked with a group from Livermore National Laboratory to measure the pressure-volume isotherm of the liquid metal up to 6 GPa at 1100 K. The volume of the sample was determined by imaging a rectangular shape of the sample with white-beam x-ray radiography, while energy-dispersive x-ray diffraction was collected to monitor the integrity of the cerium sample with respect to chemical reaction with cell assembly components.

At 1100 K, the P-V isotherm shows a clear change in its curvature, along with an inflection point indicating a decrease in the bulk modulus in moving from the γ-like liquid to an α-like liquid with pressure (Fig. 1). Advanced studies of amorphous materials and liquids are now possible with newly-commissioned capabilities at HPCAT beamline 16-BM-B.[17]

NSLS II IR Beamline Moves Forward – 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. **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 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.

Diamond Boosts Quantum Technology – New research shows that a remarkable defect in synthetic diamond produced by chemical vapor deposition allows researchers to measure, witness, and potentially manipulate electrons in a manner that could lead to new "quantum technology" for information processing. Normal computers process bits, the fundamental ones and zeros, one at a time. But in quantum computing, a "qubit" can be a one or a zero at the same time. This duplicitous state can allow multitasking at an astounding rate, which could exponentially increase the computing capacity of a tiny, tiny machine.

An "NV-" center can be created within a diamond's scaffold-like structure by replacing a missing carbon atom with a nitrogen atom (N)that has trapped an electron making the center negatively charged. Scientists can monitor the center's behavior and thereby provide a window for understanding how electrons respond to different conditions. The center has the potential to serve as a qubit in future

quantum computers. Electrons occupy different orbits around their atom and, by analogy, spin like the Earth. Carnegie scientists **Viktor Struzhkin** and **Russell J. Hemley**, along with colleagues from the Austrialian National University, the University of Melbourne, and the University of Ulm observed what happens to electrons in these NV- centers under high-pressure and normal temperatures. Their new technique offers a powerful new tool for analyzing and manipulating electrons to advance the understanding of high-pressure superconductivity, as well as magnetic and electrical properties.

The team subjected single-crystal diamonds to pressures up to 600,000 times atmospheric pressure at sea level (60 gigapascals, GPa) in a diamond anvil cell and observed how electron spin and motion were affected. They optically excited the NV- centers with light and scanned microwave frequencies in a process called optically detected magnetic resonance to determine any changes. The NV- center is very sensitive to magnetic fields, electrical fields, and stress. Until now, researchers thought that the orbits of the electrons that contribute to the defect's electronic structure and spin dynamics were localized to the area immediately surrounding the vacancy. The team found instead that the electrons also orbit more distant atoms and that the span of their orbits contract with increasing pressure.

In addition to overturning previous beliefs about the electron orbits, the researchers found a sensitive means to measure pressure. This method can detect changes in pressure of about 10 atmospheres in one second, even up to pressures of 500,000 atmospheres (50 GPa). This work demonstrates that defects in diamond have great potential as quantum sensors of high pressure phenomena and, conversely, that high pressure can be employed to study the quantum phenomena of the defects.[18]

2.3. 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.

2.3.1 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 Year 2 of the current grant period (Year 12 of the Center) 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 Jeff Montgomery
Illinois (Dlott)	Will Shaw

	Will Bassett
Yale (Lee)	Kierstin Daviau
UCLA (Kavner)	Emma Rainey
Northwestern (Jacobsen)	Yun-yuan Chang John Lazarz Josh Townsend
Washington Univ. (Schilling)	Jinhyuk Lim
Illinois (Cahill)	Greg Hohensee
Washington State (Yoo)	Gustav Borstad Dane Tomasino
Hawai'i (Dera)	Yi Hu Hannah Shelton
Utah (Miyagi)	Mike Jugle
University at Buffalo (Zurek)	Andrew Shamp
UC-Berkeley (Jeanloz)	Zack Geballe

Student Publications in 2014

Banishev, A. A., W. L. Shaw, and D. D. Dlott, Dynamics of polymer response to nanosecond shock compression, *Appl. Phys. Lett.* **104**, 101914 (2014).

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

Berg, C. M., Y. Sun, and D. D. Dlott, Picosecond dynamics of shock-compressed and flash-heated nanometer thick films of HMX, *J. Phys.: Conf. Series* **500**, 142004 (2014).

Berg, C. M., Y. Sun, and D. D. Dlott, Temperature-dependent dynamic response to flash heating of molecular monolayers on metal surfaces: Vibrational energy exchang, *J. Phys. Chem. B* **118**, 7770-7776 (2014).

Chang, Y. Y., Influence of point defects on the elastic properties of mantle minerals and superhard materials, *Ph.D. Thesis, Northwestern University* (2014).

Finkelstein, G. J., Phase transition in selected silicate minerals at high pressure and room temperature from single crystal x-ray diffraction, *Ph.D. Thesis, Princeton University* (2014).

Geballe, Z. M. and R. Jeanloz, Solid phases of FeSi to 47 GPa and 2800 K: New data, *Am. Mineral.* **99**, 720-723 (2014).

Hooper, J. T., T., A. Shamp, and E. Zurek, The composition and constitution of compressed strontium polyhydrides, *J. Phys. Chem.* **118**, 6433-6447 (2014).

Körmann, F., B. Garbowski, B. Dutta, T. Hickel, L. Mauger, B. Fultz, and J. Neugebauer, Temperature dependent magnon-phonon coupling in bcc Fe from theory and experiment, *Phys. Rev. Lett.* **113**, 165503 (2014).

Mauger, L., M. S. Lucas, J. A. Munoz, S. J. Tracy, M. Kresch, Y. Xiao, P. Chow, and B. Fultz, Nonharmonic phonons in a-iron at high temperatures, *Phys. Rev. B* **90**, 064303 (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.* **119**, 8154-8170 (2014).

Rozsa, V. F. and T. A. Strobel, Triple guest occupancy and negative compressibility in hydrogen-loaded b-hydroquinone clathrate, *J. Phys. Chem. Lett.* **5**, 1880-1884 (2014).

Shaw, W. L., A. D. Curtis, A. A. Banishev, and D. D. Dlott, Laser-driven flyer plates for shock compression spectroscopy, *J. Phys.: Conf. Series* **500**, 142011 (2014).

Shaw, W. L., D. D. Dlott, R. A. Williams, and E. L. Dreizin, Ignition of nanocomposite thermites by electric spark and shock wave, *Propell. Energ. Pyrotech.* **39**, 444-453 (2014).

Tomasino, D., M. Kim, J. Smith, and C. S. Yoo, STUDENT Pressure-induced symmetry-lowering transition in dense nitrogen to layered polymeric nitrogen (LP-N) with oclossal Raman intensity, *Phys. Rev. Lett.* **113**, 205502 (2014).

Tomasino, D. and C. S. Yoo, Probing dynamic crystal growth of compressed hydrogen using dynamic-DAC, time-resolved spectroscopy and high-speed micro-photography, *J. Phys.: Cond. Matt.* **500**, 032019 (2014).

Tracy, S. J., L. Mauger, H. J. Tan, Muñoz, Y. M. Xiao, and B. Fultz, Polaron-ion correlations in Li_xFePO_4 studied by nuclear resonant scattering at elevated pressure and temperature, *Phys. Rev. B* **90**, 094303 (2014).

Uhoya, W., D. Cargill, K. Gofryk, G. M. Tsoi, Y. K. Vohra, A. S. Sefat, and S. T. Weir, High pressure effects of the superconductivity in rare-earth-doped $CaFe_2As_2$, *High Press. Res.* **34**, 49-58 (2014).

Wenk, H. R., L. Lutterotti, P. Kaercher, W. Kanitpanyacharoen, L. Miyagi, and R. Vasin, STUDENT Rietveld texture analysis from synchrotron diffraction images: II. Complex multiphase materials and diamond anvil cell experiments, *Powder Diffr.* **29**, 220-232 (2014)

Student Presentations in 2014

Bennett, C., E. S. G. Rainey, and A. Kavner, Thermal conductivity of lower mantle minerals and heat flux across the core-mantle boundary, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Geballe, Z., A. Townley, and R. Jeanloz, How to measure heat capacity of metals at 10s to 100s of GPa, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Forouzani, N., J. Lim, J. Schilling, G. Fabbris, and Z. Fisk, High pressure study of electrical resistivity of CeB_6 to 136 GPa, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Hu, Y., P. Dera, R. T. Downs, K. Zhuravlev, R. T. Downs, and Q. Williams, New high-pressure orthorhombic Imma Ca-Fe silicate perovskite with hedenbergite composition, *COMPRES Annual Meeting* (Skamania Lodge, WA, June 16-19, 2014).

Kaluarachchi, U., V. Taufour, M. A. Tanatar, S. K. Kim, Y. Liu, T. A. Lograsso, S. L. Bud'ko, P. C. Canfield, N. Foroozani, J. Lim, and J. Schilling, Pressure dependent resistivity and magnetic measurements on superconducting KFe_2As_2, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Lazarz, J., S. M. Thomas, S. Tkachev, J. Townsend, C. Bina, and S. Jacobsen, High P-T elastic properties of OH-bearing majoritic garnet, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Lim, J., N. Foroozani, J. S. Schilling, R. Fotovat, C. Zheng, and R. Hoffmann, Hydrostatic high-pressure studies to 25 GPa on the model superconducting pnictide LaRu2P_2, *March Meeting of the American Physical Society* (Denver, CO, March 3-7, 2014).

Lim, J., N. Forouzani, J. Schilling, R. Fotovat, C. Zheng, and R. Hoffmann, Hydrostatic high-pressure studies to 25 GPa on the model superconducting pnictide $LaRu_2P_2$, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Mauger, L., M. S. Lucas, J. A. Munoz, S. J. Tracy, and B. Fultz, Anharmonic phonon entropy in alpha-Fe at elevated temperatures, *TMS 2014 Hume-Rothery Award Symposium: Thermodynamics and Kenetics of Materials* (San Diego, CA, February 18, 2014).

Miyagi, L. and M. Jugle, Deformation and transformation textures in the $NaMgF_3$ perovskite -> post-perovskite system, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Ogitsu, T., S. Hamel, A. Shamp, and E. Zurek, Phase diagram and Equation of State of Boron Carbide, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Rainey, E., C. Bennett, and A. Kavner, Thermal conductivity of lower mantle minerals and heat flux across the core-mantle boundary, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Shamp, A., Boron carbide: The evolution of structure under pressure, *Carbides, Nitrides, and Related Materials in Earth, Planetary, and Materials Science* (Davis, CA, May, 2014).

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 SiO_2 cristobalite at high temperatures and pressures, *COMPRES Annual Meeting* (Skamania Lodge, WA, June 16-19, 2014).

Tsuchiya, J., J. Townsend, T. Tsuchiya, S. Jacobsen, and C. Bina, First principles investigations of hydrous phases at the bottom of the lower mantle (Invited), *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Waszek, L., K. Arredondo, G. Finkelstein, L. Kellogg, L. Vadran, M. Li, C. Lithgow-Bertelloni, B. Romanowicz, N. Schmerr, M. Rudolph, J. Townsend, Z. Xing, and F. Yang, Slab stagnation in the lower mantle: A multidisciplinary investigation, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Zepeda-Alarcon, E., R. Lebensohn, P. Kaercher, and H. R. Wenk, Viscoplastic modeling of $MgSiO_3$ perovskite and periclase aggregates, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

As of November, 2015, 42 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)
Janelle Jenkins (Arizona State, 2009)
Lyci George (Florida International, 2010)
Michael Winterrose (Caltech, 2010)
Erin Oelker (Arizona State, 2010)
Arianna Gleason (Berkeley/Jeanloz, 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)
Chris Berg (Illinois/Dlott, 2014)
Yun-Yuan Chang (Northwestern, 2014)
Pamela Kaercher (UC-Berkeley/Wenk, 2014)
Zach Geballe (UC-Berkeley/Jeanloz, 2014)

A number of CDAC graduate students and postdoctoral fellows 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 (7)
Raja Chellappa
Wendy Mao
Nenad Velisavljevic
Janelle Jenkins
Jeffrey Carter
Kathryn Brown
Arianna Gleason

CDAC Students to Postdoctoral Positions at Other Federal Government or Government-Supported Labs or Facilities (6)
James Patterson (WSU Shock Physics)
Matt Lucas (SNS, 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 (4)
Raja Chellappa (LANL)
Nenad Velisavljevic (LANL)
Chris Seagle (SNL)
Kathryn Brown (LANL)

Carnegie Postdoctoral Fellows Obtaining Staff Positions at NNSA Labs (4)
Michael Furlanetto (LANL)
Heather Watson
Amy Lazicki (LLNL)
Luke Shulenberger (SNL)

Carnegie Postdoctoral Fellows at Other Federal Government Labs or Facilities (3)
Caitlin Murphy (AIP Congressional Fellow)
Douglas Allan Dalton (Defense Threat Reduction Agency)
Chris Berg (DOE/BES Office)

In summary, CDAC has placed 12 people in the NNSA Laboratories, an average of one person per year:

1. Mike Furlanetto
2. Raja Chellappa
3. Wendy Mao
4. Nenad Velisavljevic

5. Janelle Jenkins
6. Jeffrey Carter
7. Kathryn Brown
8. Arianna Gleason
9. Chris Seagle
10. Heather Watson
11. Amy Lazicki
12. Luke Schulenberger

2.3.2 CDAC Graduate Student NNSA Laboratory Enrichment

In the summer of 2014, CDAC supported the visits of three graduate students from Academic Partner groups to NNSA Laboratories for enrichment experiences. The students and thier advisors worked closely with NNSA Laboratory sponsors to create a project that would contribute to the students' PhD research, while at the same time offer the experience of working as a member of a research group in and NNSA Laboratory.

Figure 15*. CDAC students Andrew Shamp, Eloisa Zepeda-Alarcon, and John Lazarz present talks about their experiences working at NNSA Laboratories.*

Andrew Shamp
University at Buffalo
Advisor: Eva Zurek
Quantum Simulations Group, LLNL
Sponsors: E. Schwegler, S. Hamel, T. Ogitsu
Project: *Theoretical Studies of the Primary Hugoniot of Boron Carbide at Extreme Conditions*

Eloisa Zepeda-Alarcón
University of California-Berkeley
Advisor: Hans-Rudlof Wenk
Materials Science in Radiation and Dynamics Extremes Group, LANL
Sponsors: R. Lebensohn, C. Tom**é**
Project: *Modeling Two-Phase Deformation in Polycrystalline Aggregates Relevant to the Lower Mantle*

John Lazarz
Northwestern University
Advisor: Professor Steven Jacobsen
Shock and Detonation Physics Group, LANL
Sponsors: K. Ramos, C. Bolme
Project: *Measurement of Elasticity at Extreme Conditions*

2.3.3 Undergraduate Summer Scholars at Carnegie

CDAC supported the visits of four undergraduate students to Carnegie during 2014 for participation in the Summer Scholars Program, supervised by CDAC Coordinator Stephen Gramsch. The Carnegie Summer Scholars Program seeks to identify promising students who may not have had the opportunity to engage in research at their home institutions. At Carnegie, Summer Scholars 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.

Figure 16. *Top, Kevin Hernandez, Olivia Reyes-Becerra, and Joseph Romero. Bottom: Brooke Sherman and Brandon Wilfong.*

The following students worked with the CDAC-affiliated staff at Carnegie during the summer of 2014. 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 Na_4Si_{24} Clathrate

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 $Pb(Fe_{0.5}Nb_{0.5})O_3$ Under High Pressure and Temperature Conditions

2.3.4 SSAP Symposium 2015

The SSAP Symposium was held in Santa Fe, NM on March 11-12, 2015 At the poster session, 18 CDAC graduate students presented their work. Attending the symposium were **Will Bassett** and **Will Shaw** (Illinois), **Kierstin Daviau** (Yale), **Sakun Duwal** (Washington State), **Max Gianetta** and **Feng Lin** (Utah), **John Lazarz** (Northwestern), **Lisa Mauger** and **Fred Yang** (Caltech), **Jinhyuk Lim** (Washington University-St. Louis), **Jeff Montgomery** and **Spencer Smith** (Alabama-Birmingham), **Greg Hohensee** (Illinois), **Sulgiye Park** (Stanford), **Jeff Pigott** (Ohio State), **Andrew Shamp** (Buffalo), **Hannah Shelton** (Hawai'i), and **Eloisa Zepeda-Alarcon** (UC-Berkeley).

Eloisa Zepeda-Alarcon received a Best Poster Award for her presentation. This is the second time that she has received a Best Poster Award at this meeting. CDAC Academic Partner **Raymond Jeanloz** (UC-Berkeley) gave a presentation entitled "Journey to the Center of Jupiter: Recreating Jupiter's Core on Omega," which described recent experiments carried out at the Omega laser facility. CDAC Academic Partner **Yogesh Vohra** (Alabama-Birmingham) presented "Studies of Rare Earth Metals and Alloys Under Extreme Conditions." Former CDAC Academic Partner **Tom Duffy** (Princeton) presented "Structure of Molybdenum to 1 TPa," which also described work done at the Omega laser facility.

Student posters presented at the poster session were:

- **Will Bassett**, *Photophysics of rhodamine dyes under shock compression*
- **Kierstin Daviau**, *Inside a diamond planet: Investigating high pressure and temperature SiC*
- **Sakun Duwal**, *Pressure-induced metallization in tungsten disulfide*
- **Max Gianetta**, *Orientation relationships and stress controlled variant selection during the B1 to B2 structural transformation in NaCl*
- **Greg Hohensee**, *Inelastic thermal conductance, thermal transport in metallic silicon, and phonon scattering from magnetic defects at high pressure*
- **John Lazarz**, *Optical properties of monoclinic acetaminophen*

***Figure 18**. CDAC participants at the 2015 SSAP Symposium.*

- **Jinhyuk Lim**, *Anomalous pressure dependence of magnetic ordering temperature in Dy and Tb*
- **Feng Lin**, *Texture development at high pressure in epsilon-FeSi*
- **Lisa Mauger**, *Anharmonic phonons in bcc-Fe and Fe_3C*
- **Jeff Montgomery**, *High-temperature high-pressure phase diagram of gadolinium studied with boron-doped heater anvils*
- **Sulgiye Park**, *Complex and simple oxides under extreme environments*
- **Jeff Pigott**, *High-pressure, high-temperature equations of state using nanofabricated controlled-geometry Ni/SiO_2/Ni double hot-plate samples*
- **Andrew Shamp**, *Theoretical studies of the primary Hugoniot and solid state properties of boron carbide in extreme conditions*
- **Will Shaw**, *Shock wave energy dissipation via mechanochemistry*

- **Hannah Shelton**, *Phase transition and hydrogen bonding behavior in $Be(OH)_2$, $Zn(OH)_2$, and SiO_2 cristobalite at high temperatures and pressures*
- **Spencer Smith**, *The polymorphic behavior of paracetamol under high pressure and high temperature conditions*
- **Fred Yang**, *Phonon anharmonicity in B_2-ordered FeTi*
- **Eloisa Zepeda-Alarcon**, *Visco-plastic modeling of $MgSiO_3$ perovskite + periclase aggregates*

2.3.5 National Neutron and X-Ray Scattering School

HPCAT Beamline Scientists **Changyong Park** and **Dmitry Popov (**back row, left, and second from left, respectively in the photo) 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 HPCAT 16BM-D at the Advanced Photon Source, Argonne National Laboratory. During the two-day class, the students were provided with hands-on training for high-pressure x-ray diffraction experiments using a diamond anvil cell and a practical guide to data reduction and analysis.

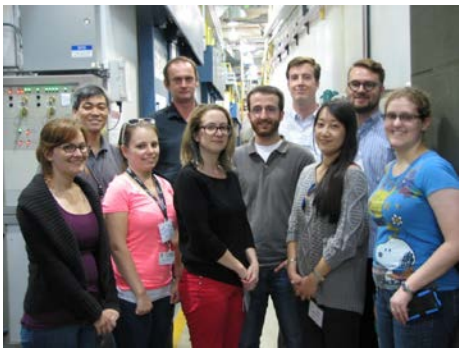

Figure 19. *Participants at the 2015 NX School.*

3. Publications and Presentations: March 2014 – February 2015

3.1 Publications

Ahart, M., A. Karandikar, S. A. Gramsch, R. Boehler, and R. J. Hemley, High P-T Brillouin scattering study of H_2O melting to 26 GPa, *High Press. Res.* **34**, 327-336 (2014).

Ahart, M., S. Kojima, Y. Yasuda, and R. J. Hemley, Successive pressure-induced structural transitions in relaxor lead indum niobate, *Ferroelectrics* **467**, 138-145 (2014).

Baker, J., R. S. Kumar, N. Velisavljevic, C. Park, C. Kenney-Benson, Y. Kono, A. Cornelius, and Y. Zhao, In situ x-ray diffraction, electrical resistivity and thermal measurements using a Paris-Edinburgh cell at HPCAT 16BM-B beamline, *J. Phys.: Conf. Series* **500**, 142003 (2014).

Bandaru, N., R. S. Kumar, J. Baker, O. Tschauner, T. Hartmann, Y. Zhao, and R. Venkat, Structural stability of WS_2 under high pressure, *Int. J. Mod. Phys. B* **28**, 1450168 (2014).

Bandaru, N., R. S. Kumar, D. Sneed, O. Tschauner, J. Baker, D. Antonio, S. N. Luo, T. Hartmann, Y. Zhao, and R. Venkat, Effect of pressure and temperature on structural stability of MoS_2, *J. Phys. Chem. C* **118**, 3230-3235 (2014).

Banishev, A. A., W. L. Shaw, and D. D. Dlott, Dynamics of polymer response to nanosecond shock compression, *Appl. Phys. Lett.* **104**, 101914 (2014).

Barabash, R. I., O. M. Barabash, D. Popov, G. Shen, C. Park, and W. Yang, Multiscale twin hierarchy in NiMnGa shape memory alloys with Fe and Cu, *Acta Mater.* **87**, 344-349 (2015).

Baumeister, J. L., E. M. Hausrath, A. A. Olsen, O. Tschauner, C. T. Adcock, and R. V. Metcalf, Biogeochemical weathering of serpentinites: An examination of incipient dissolution affecting serpentine soil formation, *Appl. Geochem.* **54**, 74-84 (2015).

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

Berg, C. M., Y. Sun, and D. D. Dlott, Picosecond dynamics of shock-compressed and flash-heated nanometer thick films of HMX, *J. Phys.: Conf. Series* **500**, 142004 (2014).
Berg, C. M., Y. Sun, and D. D. Dlott, Temperature-dependent dynamic response to flash heating of molecular monolayers on metal surfaces: Vibrational energy exchang, *J. Phys. Chem. B* **500**, 142011 (2014).
Bishop, M. M., R. S. Chellappa, Z. Liu, D. N. Preston, M. M. Sandstrom, D. M. Dattelbaum, Y. K. Vohra, and N. Velisavljevic, High pressure-temperature polymorphism of 1,1-diamino-2,2-dinitroethylene, *J. Phys.: Conf. Series* **500**, 052005 (2014).
Boulard, E., D. Pan, G. Galli, Z. Liu, and W. L. Mao, Tetrahedrally coordinated carbonates in Earth's lower mantle, *Nature Comm.* **6**, 6311 (2015).
Bowden, P. R., R. S. Chellappa, D. M. Dattelbaum, V. W. Manner, N. H. Mack, and Z. Liu, The high-pressure phase stability of 2,4,6-trinitrotoluene (TNT), *J. Phys.: Conf. Series* **500**, 052006 (2014).
Chang, Y. Y., Influence of point defects on the elastic properties of mantle minerals and superhard materials, *Ph.D. Thesis, Northwestern University* (2014).
Chang, Y. Y., S. D. Jacobsen, M. Kimura, T. Irifune, and I. Ohno, Elastic properties of transparent nano-polycrystalline diamond measured by GHz-ultrasonic interferometry and resonant sphere methods, *Phys. Earth Planet. Inter.* **228**, 47-55 (2014).
Chellappa, R., D. M. Dattelbaum, J. Coe, N. Velisavljevic, L. Stevens, and Z. Liu, Intermolecular stabilization of 3,3'-diamino-4,4'azoxyfurazen (DAAF) compressed to 20 GPa, *J. Phys. Chem. A* **118**, 5969-5982 (2014).
Chellappa, R., D. M. Dattelbaum, L. L. Daemen, and Z. Liu, High pressure spectroscopic studies of hydrazine (N_2H_4), *J. Phys.: Conf. Series* **500**, 052008 (2014).
Chen, B., Z. Li, D. Zhang, J. Liu, M. Y. Hu, J. Zhao, W. Bi, E. E. Alp, Y. Xiao, P. Chow, and J. Li, Hidden carbon in Earth's inner core revealed by shear softening in dense Fe_7C_3, *Proc. Nat. Acad. Sci.* **111**, 17755-17758 (2014).
Chen, B., K. Lutker, J. Lei, J. Yan, S. Yang, and H. K. Mao, Detecting grain rotation at the nanoscale, *Proc. Nat. Acad. Sci.* **111**, 3350-3353 (2014).
Chen, J. Y., M. Kim, C. S. Yoo, H. P. Liermann, and W. J. Evans, Time-resolved x-ray diffraction across water – ice VI/VII transformations using dynamic-DAC, *J. Phys.: Conf. Series* **500**, 142006 (2014).
Cheng, J., K. E. Kweon, S. A. Larregola, Y. Ding, Y. Shirako, L. G. Marshall, Z. Y. Li, X. Li, A. M. dos Santos, M. R. Suchomel, K. Matsubayashi, Y. Uwakoto, G. S. Hwang, J. B. Goodenough, and J. S. Zhou, Charge disproportionation and the pressure-induced insulator-metal transition in cubuc perovskite $PbCr0_3$, *Proc. Nat. Acad. Sci.* **112** (2014).
Clark, A. N., C. E. Lesher, S. D. Jacobsen, and S. Sen, Mechanisms of anomalous compressibility of vitreous silica, *Phys. Rev. B* **90**, 174110 (2014).
Cornelius, A., B. Abeln, D. Antonio, J. Baker, P. E. Kalita, and R. S. Kumar, High pressure materials physics research at UNLV, *Materials Science Forum* **783-786**, 1836 (2014).
Curtis, A. D., A. A. Banishev, W. L. Shaw, and D. D. Dlott, Laser-driven flyer plates for shock compression science: launch and target impact probed by photon Doppler velocimetry, *Rev. Sci. Instrum.* **85**, 043908 (2014).
Curtis, A. D. and D. D. Dlott, Dynamics of shocks in laser-launched flyer plates probed by photon Doppler velocimetry, *J. Phys.: Conf. Series* **500**, 192002 (2014).
Dahn, R., D. Popov, P. Schaub, P. Pattinson, D. Gromilund, U. Mader, A. Jenni, and E. Wieland, X-ray micro-diffraction studies of heterogeneous interfaces between cementitious materials and geological formations, *Phys. Chem. Earth A/B/C* **70-71**, 96-103 (2014).
Dattelbaum, D. M., R. S. Chellappa, P. R. Bowden, J. D. Coe, and M. A. Margevicius, Chemical stability of molten 2,4,6-trinitrotoluene at high pressure, *Appl. Phys. Lett.* **104**, 021911 (2014).

Dera, P., M. Manghnani, A. Hushur, Y. Hu, and S. N. Tkachev, New insights into the enigma of boron carbide inverse, *J. Solid State Chem.* **215**, 85-93 (2014).

Ding, Y., C. C. Chen, Q. Zeng, H. S. Kim, M. J. Han, M. Balasubramanian, R. Gordon, F. Li, L. Bai, D. Popov, S. M. Heald, T. Gog, H. K. Mao, and M. van Veenendaal, Novel high-pressure monoclinic metallic phase of V_2O_3, *Phys. Rev. Lett.* **112** (2014).

Doherty, M. W., V. V. Struzhkin, D. A. Simpson, L. P. McGuinness, Y. Meng, A. Stacey, T. J. Karle, R. J. Hemley, N. B. Manson, L. C. L. Hollenberg, and S. Prawer, Electronic properties and metrology of the diamond NV- center under pressure, *Phys. Rev. Lett.* **112**, 047601 (2014).

Dong, H., S. M. Dorfman, C. M. Holl, Y. meng, V. B. Prakapenka, D. He, and T. S. Duffy, Compression of lithium fluoride to 92 GPa, *High Press. Res.* **34**, 39-48 (2014).

Dong, Z. and Y. Song, Size and morphology dependent structural transformations in anatase TiO_2 nanowires under high pressures, *Can. J. Chem.* **93**, 165-172 (2015).

Efthimiopoulos, I., J. Kemichick, X. Zhou, S. V. Khare, D. Ikuta, and Y. Wang, High-pressure studies of Bi_2S_3, *J. Phys. Chem. A* **118**, 1713-1720 (2014).

Efthimiopoulos, I., A. Yaresko, V. Tsurkan, J. Deisenhofer, A. Loidl, C. Park, and Y. Wang, Pressurising the $HgCr_2Se_4$ spinel at room temperature, *Appl. Phys. Lett.* **104**, 011911 (2014).

Elkin, F. S., I. P. Zibrov, A. P. Novikov, S. S. Khasanov, V. A. Sidorov, A. E. Petrova, T. A. Lograsso, J. D. Thompson, and S. M. Stishov, Thermodynamics of the ferromagnetic phase transition in nearly half metallic CoS_2 at high pressures, *Solid State Comm.* **181**, 41-45 (2014).

Ernst, W. G. and R. J. Hemley, Francis Raymond Boyd, Jr., January 30, 1936-January 12, 2004, in *Biographical Memoirs of the National Academy of Sciences* (National Academies Press, Washington, DC, 2014).

Errandonea, D. and R. S. Kumar, High-pressure structural transformations of $PbCrO_4$ up to 51.2 GPa: An angle-dispersive synchrotron x-ray diffraction study, *Mater. Res. Bull.* **60**, 206-211 (2014).

Fabbris, G., Tuning electronic correlation with pressure, *Ph.D. Thesis, Washington University in St. Louis* (2014).

Fabbris, G., J. Lim, L. S. I. Veiga, D. Haskel, and J. S. Schilling, Electronic and structural ground state of heavy alkali metals at high pressure, *Phys. Rev. B* **91**, 085111 (2015).

Farahi, N., M. VanZant, J. Zhao, J. S. Tse, S. Prabhudev, G. A. Botton, J. R. Salvador, F. Borondics, Z. Liu, and H. Kleinke, Sb- and Bi-doped Mg2Si: Location of the dopants, micro- and nanostructures, electronic structures and thermoelectric properties, *Dalton Trans.* **43**, 14983-14991 (2014).

Feldman, J. L., D. J. Singh, and N. Bernstein, Lattice dynamical model for filled skutterudite $LaFe_4Sb_{12}$: Harmonic and anharmonic couplings, *Phys. Rev. B* **89**, 224304 (2014).

Filippousi, M., M. Angelakeris, M. Katsikini, E. Paloura, I. Efthimiopoulos, Y. Wang, D. Zamboulis, and G. Van Tendeloo, Surfactant effects on the structural and magnetic properties of iron oxide nanoparticles, *J. Phys. Chem. C* **118**, 16209-16217 (2014).

Finkelstein, G. J., Phase transition in selected silicate minerals at high pressure and room temperature from single crystal x-ray diffraction, *Ph.D. Thesis, Princeton University* (2014).

Finkelstein, G. J., P. K. Dera, S. Jahn, A. R. Oganov, C. M. Holl, Y. Meng, and T. S. Duffy, Phase transition and equation of state of foresterite to 90 GPa from single-crystal x-ray diffraction and molecular modeling, *Am. Mineral.* **99**, 35-43 (2014).

Fitzgibbons, T. C., M. Guthrie, E. S. Xu, V. H. Crespi, S. K. Davidowski, G. D. Cody, N. Alem, and J. V. Badding, Benzene-derived carbon nanothreads, *Nature Mat.* **14**, 43-47 (2015).

Foroozani, N., J. Lim, G. Fabbris, P. F. S. Rosa, Z. Fizk, and J. S. Schilling, Suppression of dense Kondo state in CeB_6 under pressure, *Physica B* **457**, 12-16 (2015).

Freiman, Y. A., S. M. Tretyak, A. Grechnev, A. F. Goncharov, and R. J. Hemley, Crystal field phenomena in hexagnal close-packed H_2 and D_2 at high pressures, *Phys. Rev. B* **90**, 024501 (2014).

Gatta, G. D., S. D. Jacobsen, P. Vignola, G. J. McIntyre, G. Guastella, and L. F. Abate, Single-crystal neutron diffraction and Raman spectroscopic study of hydroxylherderite, $CaBePO_4(OH,F)$, *Min. Mag.* **78**, 723-737 (2014).

Geballe, Z. M. and R. Jeanloz, Solid phases of FeSi to 47 GPa and 2800 K: New data, *Am. Mineral.* **99**, 720-723 (2014).

Goncharov, A. F., S. S. Lobanov, X. Tan, G. T. Hohensee, D. G. Cahill, J. F. Lin, S. M. Thomas, T. Okuchi, and N. Tomioka, Experimental study of thermal conductivity at higher pressures: Implications for the deep Earth's interior, *Phys. Earth Planet. Inter.*, doi:10.1016/j.pepi.2015.1002.1004 (2015).

Gu, T., Y. Fei, X. Wu, and S. Qin, High-pressure behavior of Fe_3P and the role of phosphorus in planetary core, *Earth Planet. Sci. Lett.* **390**, 296-303 (2014).

Haberl, B., M. Guthrie, B. D. Malone, J. S. Smith, S. V. Sinogeikin, M. L. Cohen, J. S. Williams, G. Shen, and J. E. Bradlby, Controlled formation of metastable germanium polymorphs, *Phys. Rev. B* **89**, 144111 (2014).

Harada, Y., I. Katayama, and Y. Kono, Effect of pore fluid pressure on elastic wave velocities of serpentinites, *Jpn. Mag. Min. Petrol. Sci.* **43**, 161-173 (2014).

Hooper, J. T., T., A. Shamp, and E. Zurek, Composition and constitution of compressed strontium polyhydrides, *J. Phys. Chem. C* **118**, 6433-6447 (2014).

Huang, F., Q. Zhou, L. Li, X. Huang, D. Xu, F. Li, and T. Cui, Structural transition of $MnNb_2O_6$ under quasi-hydrostatic pressure, *J. Phys. Chem. C* **118**, 19280-19286 (2014).

Huang, X., D. Duan, F. Li, Y. Huanng, L. Wang, Y. Liu, K. Bao, Q. Zhou, B. Liu, and T. Cui, Structural stability and compressive behavior of ZrH_2 under hydrostatic pressure and nonhydrostatic pressure, *RSC Adv.* **4**, 46780 (2014).

Huang, X., F. Li, Q. Zhou, G. F. Wu, Y. Huang, L. Wang, B. Li, and T. Cui, In situ synchrotron x-ray diffraction with laser-heated diamond anvil cells study of Pt up to 95 GPa and 3150 K, *RSC Adv.* **5**, 14603 (2015).

Jeffries, J. R., N. P. Butch, M. J. Lipp, J. A. Bradley, K. Kirshenbaum, S. R. Saha, J. Paglione, C. Kenney-Benson, Y. Xiao, P. Chow, and W. J. Evans, Persisntent Fe moments in the normal-state collapsed-tetragonal phase of the pressure-induced superconductor $Ca_{0.67}Sr_{0.33}Fe_2As_2$, *Phys. Rev. B* **90**, 144506 (2014).

Jeffries, J. R., L. S. I. Veiga, G. Fabbris, D. Haskel, P. Huang, N. P. Butch, S. K. McCall, K. Holliday, Z. Jenei, Y. Xiao, and P. Chow, Robust ferromagnetism in the compressed permanent magnet Sm_2Co_{17}, *Phys. Rev. B* **90**, 104408 (2014).

Jing, Z., Y. Wang, Y. Kono, T. Yu, T. Sakamaki, C. Park, M. L. Rivers, S. R. Sutton, and G. Shen, Sound velocity of Fe-S liquids at high pressure: Implications for the Moon's molten outer core, *Earth Planet. Sci. Lett.* **396**, 78-87 (2014).

Kaercher, P., Crystallographic preferred orientation and deformation of deep Earth minerals, *Ph.D. Thesis, University of California - Berkeley* (2014).

Kaercher, P., B. Militzer, and H. R. Wenk, Ab initio calculations of elastic constants of plagioclase feldspars, *Am. Mineral.* **99**, 2344-2352 (2014).

Kalita, P. E., A. Cornelius, K. E. Lipinska, S. V. Sinogeikin, R. X. L. Fischer, H., and H. Schneider, High pressure behavior of 7:4 mullite and boron-substituted mullite: Compressibility and mechanisms of amorphization, *J. Am. Ceram. Soc.* **1-10**, 34627 (2014).

Kim, J., V. V. Struzhkin, S. G. Ovchinnikov, Y. Orlov, Y. Shvyd'ko, M. H. Upton, D. Casa, A. G. Gavriliuk, and S. Sinogeikin, Pressure-induced spin transition and evolution of the electronic excitations of $FeBO_3$: Resonant inelastic x-ray scattering results, *Europhys. Lett.* **108**, 37001 (2014).

Kim, D. Y., S. Stefanoski, O. O. Kurakevych, and T. A. Strobel, Synthesis of an open-framework allotrope of silicon, *Nature Mat.* **14**, 169-173 (2015).

Kong, P. P., F. Sun, L. Y. Xing, J. Zhu, S. J. Zhang, W. M. Li, Q. Q. Liu, X. C. Wang, S. M. Feng, X. H. Yu, J. L. Zhu, R. C. Yu, W. G. Yang, G. Y. Shen, Y. S. Zhao, R. Ahuja, H. K. Mao, and C. Q. Jin, Superconductivity in strong spin orbital coupling compound Sb_2Se_3, *Sci. Reports* **4**, 6679 (2014).

Kono, Y., C. Kenney-Benson, D. R. Hummer, H. Ohfuji, C. Park, G. Shen, Y. Wang, A. Kavner, and C. E. Manning, Ultralow viscosity of carbonate melts at high pressures, *Nature Comm.* **5**, 5091 (2014).

Kono, Y., C. Park, C. Kenney-Benson, G. Shen, and Y. Wang, Toward comprehensive studies of liquids at high pressures and high temperatures: Combined structure, elastic wave velocity, and viscosity measurements in the Paris-Edinburgh cell, *Phys. Earth Planet. Inter.* **228**, 269-280 (2014).

Körmann, F., B. Garbowski, B. Dutta, T. Hickel, L. Mauger, B. Fultz, and J. Neugebauer, Temperature dependent magnon-phonon coupling in bcc Fe from theory and experiment, *Phys. Rev. Lett.* **113**, 165503 (2014).

Kothpalli, K., E. Kim, T. Kolodziej, P. F. Weck, E. E. Alp, Y. Xiao, P. Chow, C. Kenney-Benson, Y. Meng, S. N. Tkachev, A. Kozlowski, B. Lavina, and Y. Zhao, Nucleaer forward scattering and first-principles studies of the iron oxide phase Fe_4O_5, *Phys. Rev. B* **90**, 024430 (2014).

Kumar, R. S., J. J. Hamlin, M. B. Maple, Y. Zhang, C. Chen, J. Baker, A. L. Cornelius, Y. Zhao, Y. Xiao, S. V. Sinogeikin, and P. Chow, Pressure-induced superconductivity in LaFeAsO: The role of anionic height and magnetic ordering, *Appl. Phys. Lett.* **105**, 251902 (2014).

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 $EuFe_2As_2$ at low temperature and high pressures probed by resonant inelastic x-ray scattering *Appl. Phys. Lett.* **104**, 042601 (2014).

Laguna-Marco, M. A., G. Fabbris, N. M. Souza-Neto, S. S. Chikara, J. S., C. Gao, and D. Haskel, Different response of transport and magnetic properties of $BaIrO_3$ to chemical and physical pressure, *Phys. Rev. B* **90**, 014419 (2014).

Laniel, D., L. E. Downie, J. S. Smith, D. Savard, M. Murugesu, and S. Desgreniers, High pressure study of a highly energetic nitrogen-rich carbon nitride, cyanuric triazide, *J. Chem. Phys.* **141**, 234506 (2014).

Lavina, B., P. Dera, and R. T. Downs, Modern x-ray diffraction methods in mineralogy and geosciences, *Rev. Min. Geochem.* **78**, 1-31 (2014).

Lee, S. K., P. J. Eng, and H. K. Mao, Probing of pressure-induced bonding transitions in crystalline and amorphous earth materials: Insights from x-ray Raman scattering at high pressure, *Rev. Min. Geochem.* **78**, 139-174 (2014).

Li, Q., S. Li, K. Wang, J. Liu, B. Liu, K. Yang, and B. Zou, Pure hexagonal phase of EuF_3 modulated by high pressure, *J. Phys. Chem. C* **118**, 7562-7568 (2014).

Li, Z., J. Wang, L. Wang, X. Bai, H. Song, Q. Zhou, T. Wei, D. An, and B. Liu, The pressure induced amorphization and behavior of octahedron in Y_2O_3/Eu^{3+} nanotubes, *Mat. Res. Express* **1**, 025013 (2014).

Liang, Q., C. S. Yan, J. Lai, Y. F. Meng, S. Krasnicki, H. Shu, H. K. Mao, and R. J. Hemley, Large area single crystal diamond synthesis by 915 MHz microwave plasma-assisted chemical vapor deposition, *Cryst. Growth Design* **14**, 3234-3238 (2014).

Lin, J. F., E. E. Alp, and A. F. Goncharov, Raman and nuclear resonant spectroscopy in geosciences, in *Treatise on Geocshemistry, Second Edition* **207**, 195-211 (2014).

Lin, J. F., J. Wu, J. Zhu, Z. Mao, A. H. Said, B. M. Leu, J. Cheng, Y. Uwakoto, C. Jin, and J. Zhou, Abnormal elastic and vibrational behaviors of magnetite at high pressures, *Sci. Reports* **4**, 6282 (2014).

Lipp, M. J., Z. Jenei, D. Ruddle, C. Aracne-Ruddle, H. Cynn, W. J. Evans, Y. Kono, C. Kenney-Benson, and C. Park, Equation of state measurements by radiography provide evidence for a liquid-liquid phase transition in cerium, *J. Phys.: Conf. Series* **500**, 032011 (2014).

Liu, D., X. Chen, Y. Ma, Z. Liu, T. Vogt, and Y. Lee, Spectroscopic and computational characterizations of alkaline-earth- and heavy-metal-exchanged natrolites, *ChemPlusChem* **79**, 1066 (2014).

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).

Liu, J., J. F. Lin, Z. Mao, and V. B. Prakapenka, Thermal equation of state and spin transition of magnesiosiderite at high pressure and temperature, *Am. Mineral.* **99**, 84-93 (2014).

Liu, L., Y. Kono, C. Kenney-Benson, W. Yang, Y. Bi, and G. Shen, Chain breakage in liquid sulfur at high pressure and high temperature, *Phys. Rev. B* **89**, 174201 (2014).

Liu, Y., J. Wang, M. Azuma, W. L. Mao, and W. Yang, Five-dimensional visualization of phase transition in $BiNiO_3$ under high pressure, *Appl. Phys. Lett.* **104**, 043108 (2014).

Lu, X., W. Yang, Z. Quan, T. Lin, L. Bai, L. Wang, H. Fuqiang, and Y. Zhao, Enhanced electron transport in Nb-doped TiO_2 nanoparticles via pressure-induced phase transitions, *J. Am. Chem. Soc.* **136**, 419-426 (2014).

Lutterotti, L., R. Vasin, and H. R. Wenk, Rietveld texture analysis from synchrotron diffraction images: I, *Powder Diffr.* **29**, 76-84 (2014).

Ma, C., O. Tschauner, Y. Liu, J. R. Beckett, G. R. Rossman, K. Zhuravlev, V. Prakapenka, P. Dera, S. V. Sinogeikin, J. Smith, and L. Taylor, Discovery of ahrensite □-Fe_2SiO_4 and tissintite (Ca,Na,Vc)$AlSi_2O_6$: Two new high pressure minerals from the tissint martian meteorite, in *Lunar and Planetary Science Conference XXXXV* (eds. S. Mackwell and Stansbery, E.), 1222 (Lunar and Planetary Institute, 2014).

Mandal, M., F. Haso, T. Liu, Y. Fei, and K. Landskron, High yield synthesis of solution processable diamond nanocrystals, *Chem. Comm.* **50**, 11307-11310 (2014).

Manley, M. E., J. R. Jeffries, H. Lee, N. P. Butch, A. Zabalegui, and D. L. Abernathy, Multiple high-temperature transitions driven by dynamical structures in NaI, *Phys. Rev. B* **89**, 224106 (2014).

Mao, Z., J. F. Lin, J. Yang, J. Wu, H. C. Watson, Y. Xiao, P. Chow, and J. Zhao, Spin and valence states of iron in Al-bearing silicate glass at high pressures studied by synchrotron Mossbauer and x-ray emission spectroscopy, *Am. Mineral.* **99**, 415-423 (2014).

Mauger, L., M. S. Lucas, J. A. Munoz, S. J. Tracy, M. Kresch, Y. Xiao, P. Chow, and B. Fultz, Nonharmonic phonons in □-iron at high temperatures, *Phys. Rev. B* **90**, 064303 (2014).

Mkrtcheyan, V., R. Kumar, J. Baker, A. Connolly, D. Antonio, A. Cornelius, and Y. Zhao, High pressure transport and structural studies on Nb_3Ga superconductor, *Physica B* **459**, 21-23 (2015).

Najiba, S. H., Pressure and low temperature study of ammonia borane and lithium amidoborane, *Ph.D. Thesis, Florida International University* (2014).

Nakajima, Y., R. Wang, T. Metz, X. Wang, L. Wang, H. Cynn, S. T. Weir, J. R. Jeffries, and J. Paglione, High-temperature superconductivity stabilized by electride-hole interband coupling in collapsed tetragonal phase of KFe_2As_2 under high pressure, *Phys. Rev. B* **91**, 060508(R) (2015).

Naumov, I. I. and R. J. Hemley, Aromacity, closed-shell effects, and metallization of hydrogen, *Acc. Chem. Res.* **47**, 3551-3559 (2014).

Nayak, A. P., S. Bhattacharyya, J. Zhu, J. Liu, X. Wu, T. Pandey, C. Jin, A. K. Singh, D. Akinwande, and J. F. Lin, Pressure-induced semiconducting to metallic transition in multilayered molybdenum disulphide, *Nature Comm.* **5**, 3731 (2014).

Nie, Z., Y. Wang, S. Shang, Q. Zeng, Y. Ren, D. Liu, W. Yang, Y. Wang, and Z. K. Liu, Strain-induced dimensionality crossover of precursor modulations in Ni_2MnGa, *Appl. Phys. Lett.* **106**, 021910 (2015).

O'Neal, K. R., T. V. Brinzari, J. B. Wright, C. Ma, S. Giri, J. A. Schlueter, Q. Wang, P. Jena, Z. Liu, and J. L. Musfeldt, Pressure-induced magnetic crossover driven by hydrogen bonding in $CuF_2(H_2O)_2$(3-chloropyridine), *Sci. Reports* **4**, 6054 (2014).

O'Neal, K. R., Z. Liu, J. S. Miller, R. S. Fishman, and J. L. Musfeldt, Pressure-driven high to low spin transition in the bimetallic quantum magnet $[Ru_2(O_2CMe)_4]_3[Cr(CN)_6]$, *Phys. Rev. B.* **90**, 104301 (2014).

Palasyuk, T., I. A. Troyan, M. Eremets, V. Drozd, S. Medvedev, P. Zaleski-Ejgierd, E. Magos-Palasyuk, H. Wang, S. A. Bonev, D. Dudenko, and P. Naumov, Ammonia as a case study for the spontaneous ionization of a simple hydrogen-bonded compound, *Nature Comm.* **5**, 3460 (2014).

Pandey, K. K., J. Gyanchandani, M. Somayazulu, G. K. Gey, S. M. Sharma, and S. K. Sikka, Reinvestigation of high pressure polymorphism in hafnium metal, *J. Appl. Phys.* **115**, 233513 (2014).

Park, S. Y., M. Lang, C. L. Tracy, J. Zhang, F. W. Zhang, C. Trautmann, P. Kluth, M. D. Rodriguez, and R. C. Ewing, Swift heavy ion irradiation-induced amorphization of $La_2Ti_2O_7$, *Nucl. Instr. Meth. Phys. Res. B* **326**, 145-149 (2014).

Potter, R., M. Somayazulu, G. Cody, and R. J. Hemley, Raman spectroscopy, x-ray diffraction, and hydrogenation thermochemistry of N,N,N,N-tetramethylcyclotriborazane under pressures, *J. Phys. Chem. C* **118**, 9871-9879 (2014).

Potter, R. G., M. Somayaulu, G. Cody, and R. J. Hemley, High pressure equilibria of dimethylamine borane, dihydridobis(dimethylamine)boron(III) tetrahydridoborate(III), and hydrogen, *J. Phys. Chem. C* **118**, 7280-7287 (2014).

Pravia, M., D. Sneed, M. White, and Y. Wang, Note: Loading method of molecular fluorine using x-ray induced chemistry, *Rev. Sci. Instrum.* **85**, 086110 (2014).

Pravica, M., B. Hulsey, L. Bai, D. Sneed, Q. Smith, and G. Guardala, Studies in useful hard x-ray photochemistry: Decomposition of potassium halates, *J. Phys.: Conf. Series* **500**, 022009 (2014).

Pravica, M., D. Sneed, Y. Wang, Q. Smith, and G. Subrahmanyam, Carbon tetrachloride under extreme conditions, *J. Chem. Phys.* **140**, 194503 (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.* **119**, 8154-8170 (2014).

Rozsa, V. F. and T. A. Strobel, Triple guest occupancy and negative compressibility in hydrogen-loaded ß-hydroquinone clathrate, *J. Phys. Chem. Lett.* **5**, 1880-1884 (2014).

Sakamaki, T., Y. Kono, Y. Wang, C. Park, T. Yu, Z. Jing, and G. Shen, Contrasting sound velocity and intermediate-range structural order between polymerized and depolymerized silicate glasses under pressure, *Earth Planet. Sci. Lett.* **391**, 288-295 (2014).

Samudrala, G. K., G. M. Tsoi, S. T. Weir, and Y. K. Vohra, Structural and magnetic phase transitions in gadolinium under high pressures and low temperatures, *High Press. Res.* **34**, 385-391 (2014).

Saxena, S. K. and R. Hrubiak, Mapping the nebular condensates and the chemical composition of the terrestrial planets, *Earth Planet. Sci. Lett.* **393**, 113-119 (2014).

Schmandt, B., S. D. Jacobsen, T. W. Becker, Z. Liu, and K. G. Dueker, Dehydration melting at the top of the lower mantle, *Science* **344**, 1265-1268 (2014).

Seoung, D., Y. Lee, H. Cynn, C. Park, K. Y. Choi, D. A. Blom, W. J. Evans, C. C. Kao, T. Vogt, and Y. Lee, Irreversible xenon insertion into a small-pore zeolite at moderate pressures and temperatures, *Nature Chem.* **6**, 835-839 (2014).

Shaw, W. L., A. D. Curtis, A. A. Banishev, and D. D. Dlott, Laser-driven flyer plates for shock compression spectroscopy, *J. Phys.: Conf. Series* **500**, 142011 (2014).
Shaw, W. L., D. D. Dlott, R. A. Williams, and E. L. Dreizin, Ignition of nanocomposite thermites by electric spark and shock wave, *Propell. Energ. Pyrotech.* **39**, 444-453 (2014).
Shaw, W. L., R. A. Williams, E. L. Dreizin, and D. D. Dlott, Using laser-driven flyer plates to study the shock initiation of nanoenergetic materials, *J. Phys.: Conf. Series* **500**, 182010 (2014).
Shen, G. and Y. Wang, High-pressure apparatus integrated with synchrotron radiation, *Rev. Min. Geochem.* **78**, 745-777 (2014).
Smith, R. F., J. H. Eggert, R. Jeanloz, T. S. Duffy, D. G. Braun, J. R. Patterson, R. E. Rudd, J. Biener, A. E. Lazicki, A. V. Hamza, J. Wang, T. Braun, L. X. Benedict, P. M. Celliers, and G. W. Collins, Ramp compression of diamond to five terapascals, *Nature* **511**, 330-333 (2014).
Smith, S. J., M. M. Bishop, J. M. Montgomery, T. P. Hamilton, and Y. K. Vohra, Polymorphism in paracetamol: Evidence of additional forms IV and V at high pressure, *J. Phys. Chem. A* **118**, 6068-6077 (2014).
Spice, H., C. Sanloup, B. Cochain, C. de Grouchy, and Y. Kono, Viscosity of liquid fayalite up to 9 GPa, *Geo. Cosmo.* **148**, 219-227 (2015).
Stemshorn, A., Devitrification of iron based metallic glasses at high pressures and temperatures, *Ph.D. Thesis, University of Alabama at Birmingham* (2014).
Stinton, G. W., S. G. MacLeod, H. Cynn, D. Errandonea, W. J. Evans, J. E. Proctor, Y. Meng, and M. I. McMahon, Equation of state and high-pressure/high-temperature phase diagram of magnesium, *Phys. Rev. B* **90**, 134105 (2014).
Strobel, T. A., O. O. Kurakevych, D. Y. Kim, Y. Le Godec, W. Crichton, J. Guignard, N. Guignot, G. D. Cody, and A. R. Oganov, Synthesis of □-Mg_2C_3: A monolithic high-pressure polymorph of magnesium sesquicarbide, *Inorg. Chem.* **53**, 7020-7027 (2014).
Sun, Y., L. Wang, Y. Liu, and Y. Ren, Birnessite-type MnO_2 nanosheets with layered structurs under high pressure: Elimination of crystalline stacking faults and oriented laminar assembly, *Small* **11**, 300-305 (2015).
Tochigi, E., E. Zepeda-Alarcon, H. R. Wenk, and A. M. Minor, In situ TEM observations of plastic deformation in quartz crystals, *Phys. Chem. Minerals* **41**, 757-765 (2014).
Tomasino, D., M. Kim, J. Smith, and C. S. Yoo, Pressure-induced symmetry-lowering transition in dense nitrogen to layered polymeric nitrogen (LP-N) with oclossal Raman intensity, *Phys. Rev. Lett.* **113**, 205502 (2014).
Tomasino, D. and C. S. Yoo, Probing dynamic crystal growth of compressed hydrogen using dynamic-DAC, time-resolved spectroscopy and high-speed micro-photography, *J. Phys.: Conf. Series* **500**, 032019 (2014).
Tracy, C. L., J. M. Pray, M. Lang, D. Popov, C. Park, C. Trautmann, and R. C. Ewing, Defect accumulation in ThO_2 irradiated with switft heavy ions, *Nucl. Instr. Meth. Phys. Res. B* **326**, 169-173 (2014).
Tracy, S. J., L. Mauger, H. J. Tan, Muñoz, Y. M. Xiao, and B. Fultz, Polaron-ion correlations in Li_xFePO_4 studied by nuclear resonant scattering at elevated pressure and temperature, *Phys. Rev. B* **90**, 094303 (2014).
Tracy, C. L., M. Lang, J. M. Pray, F. W. Zhang, D. Popov, C. Park, C. Trautmann, M. Bender, D. Severin, V. A. Skuratov, and R. C. Ewing, Redox response of actinide materials to highly ionizing radiation, *Nature Comm.* **6**, 6133 (2015).
Uhoya, W., D. Cargill, K. Gofryk, G. M. Tsoi, Y. K. Vohra, A. S. Sefat, and S. T. Weir, High pressure effects of the superconductivity in rare-earth-doped $CaFe_2As_2$, *High Press. Res.* **34**, 49-58 (2014).
Uhoya, W., G. M. Tsoi, Y. K. Vohra, A. S. Sefat, and S. T. Weir, Pressure-induced superconductivity and structural transitions in $Ba(Fe_{0.9}Ru_{0.1})_2As_2$, *Euro. Phys. J. B* **87**, 68 (2014).

Velisavljevic, N., M. K. Jacobsen, and Y. K. Vohra, Structural phase stability in nanocrystalline titanium to 161 GPa, *Mat. Res. Express* **1**, 035044 (2014).
Velisavljevic, N., S. V. Sinogeikin, R. Saavedra, R. Chellappa, A. Rothkirch, D. M. Dattelbaum, Z. Konopkova, H. P. Liermann, M. Bishop, G. M. Tsoi, and Y. K. Vohra, Time-resolved x-ray diffraction and electrical resistance measurements of structural phase transitions in zirconium, *J. Phys.: Conf. Series* **500**, 032020 (2014).
Vilaplanna, R., R. Lacomba-Perales, O. Gomis, D. Errandonea, and Y. Meng, Quasi-hydrostatic x-ray powder diffraction study of the low- and high-pressure phases of $CaWO_4$ up to 28 GPa, *Solid State Sci.* **36**, 16-23 (2014).
Wang, K., J. Liu, K. Yang, B. Liu, and B. Zou, High-pressure-induced reversible phase transition in sulfamide, *J. Phys. Chem. C* **118**, 18640-18645 (2014).
Wang, S., A. F. Kemper, M. Baldini, M. C. Shapiro, S. C. Riggs, Z. Zhao, Z. Liu, T. P. Devereaux, T. H. Geballe, I. R. Fisher, and W. L. Mao, Bandgap closure and reopening in $CsAuI_3$ at high pressure, *Phys. Rev. B* **89**, 245109 (2014).
Wang, S., X. Yu, J. Zhang, Y. Zhang, L. Wang, K. Leinenweber, H. Xu, D. Popov, C. Park, W. Yang, D. He, and Y. Zhao, Crystal structures, elastic properties, and hardness of high-pressure synthesized CrB_2 and CrB_4, *J. Superhard Mater.* **36**, 279-287 (2014).
Wang, S., J. Zhang, J. Yan, X. J. Chen, V. V. Struzhkin, W. Tabis, N. Barisic, M. K. Chan, C. Dorow, X. Zhao, M. Greven, W. L. Mao, and T. Geballe, Strain derivatives of T_c in $HgBa_2CuO_{4+\square}$: The CuO_2 plane alone is not enough, *Phys. Rev. B* **89**, 024515 (2014).
Wang, W., S. Wang, D. He, and J. Xu, Pressure induced phase transition of $PbNiO_3$ from $LiNbO_3$-type to perovskite, *Solid State Comm.* **196**, 8-12 (2014).
Wang, X., M. Misek, M. K. Jacobsen, and K. V. Kamenev, Use of an advanced composite material in construction of a high pressure cell for magnetic ac susceptibility measurements, *High Press. Res.* **34**, 371-384 (2014).
Wang, Y., T. Sakamaki, L. B. Skinner, Z. Jing, T. Yu, Y. Kono, C. Park, G. Shen, M. L. Rivers, and S. R. Sutton, Atomistic insight into viscosity and density of silicate melts under pressure, *Nature Comm.* **5**, 3241 (2014).
Wang, Y. and G. Shen, High-pressure experimental studies on geo-liquids using synchrotron radiation at the Advanced Photon Source, *J. Earth. Sci.* **25**, 939-958 (2014).
Wenk, H. R., L. Lutterotti, P. Kaercher, W. Kanitpanyacharoen, L. Miyagi, and R. Vasin, Rietveld texture analysis from synchrotron diffraction images: II. Complex multiphase materials and diamond anvil cell experiments, *Powder Diffr.* **29**, 220-232 (2014).
Wong, J., A. Mailman, K. Lekin, S. M. Winter, W. Yong, J. Zhao, S. Garimella, J. Tse, R. A. Secco, S. Desgreniers, Y. Ohishi, F. Borondics, and R. T. Oakley, Pressure induced phase transition and metallization of a neutral radical conductor, *J. Am. Chem. Soc.* **136**, 1070-1081 (2014).
Wu, J. J., J. F. Lin, X. C. Wang, Q. Q. Liu, J. L. Zhu, Y. M. Xiao, P. Chow, and C. Q. Jin, Magnetic and structural transitions of $SrFe_2As_2$ at high pressure and low temperature, *Sci. Reports* **4**, 3685 (2014).
Wu, X., F. Ma, C. Ma, H. Cui, Z. Liu, H. Zhu, X. Wang, and Q. Cui, Pressure-driven variations of hydrogen bonding energy in ammonium azide (NH4N3): IR absorption and Raman scattering studies, *J. Chem. Phys.* **141**, 024703 (2014).
Xi, X., X. G. He, F. Guan, W. Ku, Z. Liu, R. D. Zhong, J. A. Schneeloch, T. S. Liu, G. D. Gu, D. Xu, Z. Chen, X. G. Hong, and G. L. Carr, Bulk signatures of pressure-induced band inversion of topological phase transitions in $Pb_{1-x}Sn_xSe$, *Phys. Rev. Lett.* **113**, 096401 (2014).
Xi, X., C. Ma, Z. Liu, Z. Chen, W. Ku, H. Berger, C. D. Martin, D. B. Tanner, and G. L. Carr, Signatures of a pressure-induced topological quantum phase transition in BiTeI, *Phys. Rev. Lett.* **111**, 155701 (2014).

Xie, M., B. Winkler, Z. Mao, R. B. Kaner, A. Kavner, and S. H. Tolbert, Raman scattering of superhard rhenium diboride under high pressure, *Appl. Phys. Lett.* **104**, 011904 (2014).

Yan, H., C. Park, G. Ahn, S. M. Hong, D. T. Keane, C. Kenney-Benson, P. Chow, Y. Xiao, and G. Shen, Termination and hydration of forsteritic olivine (0 1 0) surface, *Geochim. Cosmochim. Acta* **145**, 268-280 (2014).

Yang, F., Y. Lin, J. E. P. Dahl, R. M. K. Carlson, and W. L. Mao, High pressure Raman and x-ray diffraction study of [121] tetramantane, *J. Phys. Chem. C* **118**, 7683-7689 (2014).

Yang, F., Y. Lin, J. E. P. Dahl, R. M. K. Carlson, and W. L. Mao, Deviatoric stress-induced phase transitions in diamantane, *J. Chem. Phys.* **141**, 154305 (2014).

Yang, H., L. Martinelli, F. Tasso, A. R. Sprocati, F. Pinzari, Z. Liu, R. T. Downs, and H. J. Sun, A new biogenic, struvite-related phosphate, the ammonium-analog of hazenite (NH4)$NaMg_2(PO_4)_2 \cdot 14H_2O$, *Am. Mineral.* **99**, 1761-1766 (2014).

Yang, W., F. J. Jia, L. Y. Tang, L. J. Li, Z. A. Xu, and X. J. Chen, Structure feature controlling superconductivity in compressed $BaFe_2As_2$, *J. Appl. Phys.* **115**, 083915 (2014).

Ye, Y., C. Gu, S. H. Shim, Y. Meng, and V. Prakapenka, The postspinel boundary in pyrolitic compositions determined in the laser-heated diamond anvil cell, *Geophys. Res. Lett.* **41**, 3833-3841 (2014).

Yu, Z., L. Wang, L. Wang, H. Liu, J. Zhao, C. W. Li, S. V. Sinogeikin, W. Wu, J. Luo, N. Wang, K. Yang, Y. Zhao, and H. K. Mao, Conventional empirical law reverses in the phase transitions of 122-type iron-based superconductors, *Sci. Reports* **4**, 7172 (2014).

Zeng, Q., Y. Kono, Y. Li, Z. Zeng, J. Wang, S. V. Sinogeikin, C. Park, Y. Meng, W. Yang, H. K. Mao, and W. L. Mao, Universal fractional noncubic power law for density of metallic glasses, *Phys. Rev. Lett.* **112**, 185502 (2014).

Zepeda-Alarcon, E., H. Nakotte, A. F. Gualtieri, G. King, K. Page, S. C. Vogel, H. W. Wang, and H. R. Wenk, Magnetic and nuclear structure of goethite α-FeOOH: A neutron diffraction study, *J. Appl. Cryst.* **47**, 1983-1991 (2014).

Zha, C. S., R. E. Cohen, H. K. Mao, and R. J. Hemley, Raman measurements of phase transitions in dense solid hydrogen and deuterium to 325 GPa, *Proc. Nat. Acad. Sci.* **111**, 4792-4797 (2014).

Zhang, F. X., M. Lang, C. Tracy, R. C. Ewing, D. J. Gregg, and G. R. Lumpkin, Incorporation of uranium in pyrochlore oxides and pressure-induced phase transitions, *J. Solid State Chem.* **219**, 49-54 (2014).

Zhang, J. S., S. Shieh, J. D. Bass, P. Dera, and V. Prakapenka, High-pressure single-crystal elasticity study of CO_2 across phase I-III transition, *Appl. Phys. Lett.* **104**, 141901 (2014).

Zhang, L., Y. Meng, W. Yang, L. Wang, W. L. Mao, Q. S. Zeng, J. S. Jeong, A. J. Wagner, K. A. Mkhoyan, W. Liu, R. Xu, and H. K. Mao, Disproportionation of (Mg,Fe)SiO_3 perovskite in Earth's deep lower mantle, *Science* **344**, 877-882 (2014).

Zhang, S., X. Wang, J. Zhu, C. Jin, H. Gong, and L. Li, The microstructure and ferroelectricity of $BiScO_3$-$PbTiO_3$ nanoceramics at morphotropic phase boundaries, *Scripta Mater.* **82**, 45-48 (2014).

Zhang, D., J. M. Jackson, J. Zhao, W. Sturhahn, E. E. Alp, T. S. Toellner, and M. Y. Hu, Fast temperature spectrometer for samples under extreme conditions, *Rev. Sci. Instrum.* **86**, 013105 (2015).

Zhao, Z., C. Meng, P. Li, W. ZHu, Q. Wang, Y. Ma, G. Shen, L. Bai, H. He, D. He, D. Yu, J. He, B. Xu, and Y. Tian, Carbon coated face-centered cubic Ru-C nanoalloys, *Nanoscale* **6**, 10370-10376 (2014).

Zhao, Z., S. Wang, A. R. Oganov, P. N. Chen, Z. Liu, and W. L. Mao, Tuning the crystal structure and electronic states of Ag_2Se: Structure transitions and metallization under pressure, *Phys. Rev. B* **89**, 180102 (2014).

Zhao, Z., S. Wang, T. F. Qi, Q. Zeng, S. Hirai, P. P. Kong, L. Li, C. Park, S. J. Yuan, C. Q. Jin, G. Cao, and W. L. Mao, Pressure induced second-order structural transition in $Sr_3Ir_2O_7$, *J. Phys.: Cond. Matt.* **26**, 215402 (2014).

Zhao, Z., E. F. Wang, H. Yan, Y. Kono, B. WEn, L. Bai, F. Shi, J. Zhang, C. Kenney-Benson, C. Park, Y. Wang, and G. Shen, Nanoarchitectured materials composed of fullerene-like spheroids and disordered graphene layers with tunable mechanical properties, *Nature Comm.* **6**, 6212 (2015).

Zhou, L., N. Shinde, A. Hu, C. Cook, M. Murugesu, and Y. Song, Structural tuning of energetic material bis(1*H*-tetrazol-5-yl)amine monohydrate under pressure probed by vibrational spectroscopy and x-ray diffraction, *J. Phys. Chem. C* **118**, 26504-26512 (2014).

Zhou, M., K. Wang, Z. Men, C. Sun, Z. Li, B. Liu, G. Zou, and B. Zou, Pressure-induced isostructural phase transition of a metal-organin framework Co_2(4,4'-bpy)$_3$(NO_3)$_4$·xH_2O, *Cryst. Eng. Comm.* **16**, 4084-4087 (2014).

3.2 Presentations

Ahart, M., R. E. Cohen, and R. J. Hemley, Pressure-induced transitions in ferroelectric single-crystal $PbZr_{0.54}Ti_{0.46}O_3$, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Ali, S. J., R. Smith, D. Erskine, J. Eggert, P. Celliers, G. W. Collins, and R. Jeanloz, Two-dimensional imaging velocimetry of heterogeneous flow and brittle failure in diamond, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Benitez-Perez, J. M., J. Gomez Barreiro, H. R. Wenk, S. Vogel, Y. Soda, M. Voltolini, and J. Martinez-Catalan, Quantitative texture analysis of talc in mantle hydrated mylonites, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Bennett, C., E. S. G. Rainey, and A. Kavner, Thermal conductivity of lower mantle minerals and heat flux across the core-mantle boundary, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Bennett, N. and Y. Fei, Element redistribution in Fe-Ni-O alloys by a thermal gradient: Implications for siderophile element partitioning during core formation and crystallization, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Bian, H., Z. Mao, J. F. Lin, J. Yang, J. Liu, H. Watson, H. Chen, J. Shim, V. Prakapenka, Y. Xiao, and P. Chow, (Fe,Al)-bearing post-perovskite in the Earth's lower mantle, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Butch, N. P., J. Jeffries, P. Syers, J. Paglione, Y. Xiao, and P. Chow, Valence and moment of Sm in SmB_6 under pressure, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Cahill, D., J. Huang, W. Wang, and C. Murphy, Resonant secondary light emission from plasmonic Au nanostructures at high electron temperatures created by pulsed laser excitation, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 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).

Chen, H., S. H. Shim, K. Leinenweber, Y. Meng, and V. Prakapenka, Crystal structure of calcium silicate perovskite synthesized under water saturated conditions at mantle related pressure-temperature, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Chen, J. Y., C. S. Yoo, M. Kim, H. P. Liermann, H. Cynn, Z. Jenei, and W. Evans, Solidification and fcc- to metastable hcp- phase transition in krypton under modulating dynamic pressures, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Chen, X. J., Y. H. Zhou, J. J. Ying, T. Muramatsu, V. Struzhkin, H. K. Mao, Z. A. Xu, X. H. Chen, G. Y. Xu, and G. D. Gu, Iron-based superconductors under heavy compression

after destruction of superconductivity, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).
Clark, A., C. Lesher, S. Jacobsen, T. Yu, and Y. Wang, Volumetric and elastic properties of basalt at high pressure by x-ray microtomography and GHz-ultrasonic interferometry, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).
Cohen, R. E., I. I. Naumov, and R. J. Hemley, Optical signature of metallization of hydrogen, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).
Collins, G. W., et al., Exotic behavior of matter in the deep interiors of exoplanets, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).
Cottaar, S., M. Li, A. McNamara, B. Romanowicz, and H. R. Wenk, The role of post-perovskite in explaining observations of seismic anisotropy (Invited), *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).
Diamond, M., S. J. Ali, J. Eggert, R. Jeanloz, G. W. Collins, and R. McWilliams, Investigating metallization in shock-compressed alkali halides, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).
Dlott, D. D., SFG studies of buried electrochemical interfaces (invited), *American Chemical Society National Meeting* (Dallas, TX, March, 2014).
Dlott, D. D., Probing dynamic materials interfaces using nonlinear coherent vibrational spectroscopy, *AFOSR Dynamic Interfaces Workshop* (Arlington, VA, March 2014).
Dlott, D. D., Probing shocked microstructured energetic materialss, *AFOSR Dynamic Interfaces Workshop* (Arlington, VA, March 2014).
Dlott, D. D., Vibrational energy transfer on surfaces and in liquids, *MIT Modern Optics and Spectroscopy Seminar* (Cambridge, MA, April, 2014).
Driver, K., S. Zhang, B. Militzer, and R. E. Cohen, Quantum Monte Carlo simulations of a single iron impurity in MgO, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).
Fei, Y., L. Han, N. Bennett, M. Hou, Y. Kuwayama, and H. Huang, Multiple experimental efforts to understand the structure and dynamics of Earth's core (Invited), *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).
Finkelstein, G., P. Dera, and T. Duffy, High-pressure phase of cordierite from single-crystal x-ray diffraction to 15 GPa, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).
Forouzani, N., J. Lim, J. Schilling, G. Fabbris, and Z. Fisk, High pressure study of electrical resistivity of CeB_6 to 136 GPa, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).
Fultz, B., Entropy, phonons, and nuclear resonant x-ray scattering, *SLAC Photon Science Seminar Series* (Stanford, CA, September 3, 2014).
Geballe, Z., A. Townley, and R. Jeanloz, How to measure heat capacity of metals at 10s to 100s of GPa, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).
Godwal, B., F. Gonzalez-Cataldo, and R. Jeanloz, Siulating ramp compression of diamond, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).
Gomez Barreiro, J., M. Voltolini, J. Martinez-Catalan, J. M. Benitez-Perez, R. Diez-Fernandez, H. R. Wenk, S. Vogel, and L. Mancini-Elettra, Quantitative fabric analysis of eclogite facies mylonites: texture and microtomography, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).
Han, L., Y. Fei, and L. Zhang, Behavior of K in eclogite from subducted slab at pressures from 4 to 10 GPa, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).
Hemley, R. J., Next generation materials: Challenges and opportunities of extreme environments (invited), *ARL Colloquium* (Aberdeen Proving Ground, Aberdeen, MD, April 9, 2014).
Hu, Y., P. Dera, R. T. Downs, K. Zhuravlev, R. T. Downs, and Q. Williams, New high-pressure orthorhombic Imma Ca-Fe silicate perovskite with hedenbergite composition, *COMPRES Annual Meeting* (Skamania Lodge, WA, June 16-19, 2014).

Hummer, D., A. Kavner, C. Manning, C. Park, Y. Kono, and C. Kenney-Benson, Viscosity of carbonate-silicate melts using ultra-high resolution falling sphere viscometry, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Jackson, J., A. Wolf, J. Wicks, N. Solomatova, D. Bower, D. Dun, W. Sturhahn, P. Dera, and V. Prakapenka, Sound velocities and equations of state for lower mantle phases: Implications for deep mantle structures (Invited), *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Jeanloz, R. and M. Ishii, Seismological constraints on lower-mantle convection, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Jeffries, J., N. P. Butch, Y. K. Vohra, and S. T. Weir, Pressure evolution of electrical transport in the 3D topological insulator $(Bi,Sb)_2(Te,Se)_3$, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Kaluarachchi, U., V. Taufour, M. A. Tanatar, S. K. Kim, Y. Liu, T. A. Lograsso, S. L. Bud'ko, P. C. Canfield, N. Foroozani, J. Lim, and J. Schilling, Pressure dependent resistivity and magnetic measurements on superconducting KFe_2As_2, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Kavner, A. and M. Armentrout, High-pressure, high-temperature equations of state for Fe, Ni, andCo silicates, oxides, and metals: Constructing a deep earth electrochemical series, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Lavina, B. and Y. Meng, Complexity of high-pressure orthorhombic iron oxides, the characterization of Fe_5O_6, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Lazarz, J., S. M. Thomas, S. Tkachev, J. Townsend, C. Bina, and S. Jacobsen, High P-T elastic properties of OH-bearing majoritic garnet, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Li, D., P. Zhao, N. Gunning, D. Johnson, J. C. Zhao, and D. Cahill, Measurement of surface acoustic wave velocity using phase shift mask and application on thin film of thermoelectric material, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Lim, J., N. Foroozani, J. S. Schilling, R. Fotovat, C. Zheng, and R. Hoffmann, Hydrostatic high-pressure studies to 25 GPa on the model superconducting pnictide LaRu2P_2, *March Meeting of the American Physical Society* (Denver, CO, March 3-7, 2014).

Lim, J., N. Forouzani, J. Schilling, R. Fotovat, C. Zheng, and R. Hoffmann, Hydrostatic high-pressure studies to 25 GPa on the model superconducting pnictide $LaRu_2P_2$, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Lin, Y., R. E. Cohen, K. Driver, B. Militzer, L. Shulenburger, and J. Kim, Quantum Monte Carlo calculation for the equation of state of $MgSiO_3$ perovskite at high pressures, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Liu, H., Y. Fei, L. Han, Y. Kono, M. Hou, Z. Zhao, and J. Du, Viscosity measurements of eclogite melt up to 5.6 GPa and 2000 K, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Liu, J., J. Li, and D. Ikuta, "Invar"-like behavior in compressed Fe_7C_3 with implication for deep carbon cycle, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Mandal, S., R. E. Cohen, and K. Haule, A DFT+DMFT investigation on electron-phonon coupling in FeSe, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Mao, W., Y. Lin, Y. Liu, C. Shi, and W. Yang, 3D spectroscopic x-ray imaging with nanoscale resolution at extreme conditions (Invited), *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Marquardt, H., L. Miyagi, S. Speziale, H. P. Liermann, S. Merkel, and C. Tomé, Deformation of (Mg,Fe)O ferropericlase to temperatures of 1150 K and pressures of 96 GPa: Implications for mantle flow and seismic anisotropy (Invited), *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Miller, R., J. Jackson, W. Sturhahn, J. Zhao, and C. Murphy, Sound velocities of iron-nickel and iron-nickel-silicon alloys at high pressure, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Millot, M., S. Hammel, J. Rygg, R. Jeanloz, and G. W. Collins, Optical properties of superionic water at 2 Mbar, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Miyagi, L. and M. Jugle, Deformation and transformation textures in the $NaMgF_3$ perovskite -> post-perovskite system, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Muramatsu, T., V. Struzhkin, and L. Gasparov, Electrical resistivity study of Magnetite under high pressure, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Naumov, I. I., R. E. Cohen, and R. J. Hemley, Graphene physics and insulator-metal transition in compressed hydrogen, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Nisr, C., S. H. Shim, K. Leinenweber, R. Hervig, V. Prakapenka, and Y. Meng, Water in Al-free stishovite up to 65 GPa and 200 K, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Ogitsu, T., S. Hamel, A. Shamp, and E. Zurek, Phase diagram and Equation of State of Boron Carbide, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

O'Neal, K., T. Brinzaria, J. Wright, J. Musfeldt, S. Giri, Q. Wang, P. Jena, J. Schlueter, and Z. Liu, Pressure-induced magnetic crossover driven by hydrogen bonding in $CuF_2(H_2O)_2$(3-chloropyridine), *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Palaich, S., C. Tulk, J. Molaison, A. Makhluf, M. Guthrie, A. Kavner, and C. Manning, Structure and thermal behavior of CO_2-IV at 18 GPa from 300-625 K, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Pravica, M., D. Popov, S. Sinogeikin, D. Sneed, Q. Smith, and G. Guardala, X-ray induced mobility of molecular oxygen at extreme conditions, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Rainey, E., C. Bennett, and A. Kavner, Thermal conductivity of lower mantle minerals and heat flux across the core-mantle boundary, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Schilling, J. S., Contrasting effects of extreme pressure on highly correlated electron behavior (invited), *International Workshop on Pressure and Strain Effects in Correlated Electron Materials* (Dresden, Germany, October 6-10, 2014).

Schmandt, B., S. Jacobsen, T. Becker, Z. Liu, and K. Dueker, Dehydration melting in the top of the lower mantle (Invited), *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Shamp, A., Boron carbide: The evolution of structure under pressure, *Carbides, Nitrides, and Related Materials in Earth, Planetary, and Materials Science* (Davis, CA, May, 2014).

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 SiO_2 cristobalite at high temperatures and pressures, *COMPRES Annual Meeting* (Skamania Lodge, WA, June 16-19, 2014).

Shibazaki, Y., Y. Kono, Y. Fei, and G. Shen, Structure measurement of liquid Fe-C alloys at high pressure, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Sinogeikin, S., J. Smith, C. Lin, L. Bai, E. Rod, and G. Shen, Elasticity and anelasticity of materials from time-resolved x-ray diffraction, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Smart, T., M. Diamond, E. O'Bannon, J. Yuan, S. Stackhouse, B. Godwal, R. Jeanloz, and Q. Williams, $PbCl_2$ and $SnCl_2$ at high-pressures as analogs for SiO_2 metallization, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Stagno, V., K. Crispin, A. Shahar, and Y. Fei, Growht kinetics of a reaction rim between iron and graphite/diamond and the carbon diffusion mechanism at high pressure and temperature, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Tan, X., A. F. Goncharov, V. Struzhkin, and X. Chen, Study electron-phonon interactions under high pressures by ultrafast time-resolved spectroscopy, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Thomas, S. M., S. Jacobsen, C. Bina, P. Reichart, M. Moser, G. Dollinger, and E. Hauri, Water in olivine and its high-pressure polymorphs, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Tsuchiya, J., J. Townsend, T. Tsuchiya, S. Jacobsen, and C. Bina, First principles investigations of hydrous phases at the bottom of the lower mantle (Invited), *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Wang, S., J. Zhang, X. J. Chen, V. Struzhkin, W. Tabis, N. Barisic, M. Chan, C. Dorow, X. Zhao, M. Greven, W. Mao, and T. Geballe, The strain derivatives of T_c in $HgBa_2CuO_{4+\delta}$: CuO_2 plane alone is not enough, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Wang, X., N. Coates, R. Segalman, and D. Cahill, Lorenz number of conducting PEDOT:PSS, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Wang, Y., T. Yu, C. Prescher, V. Prakapenka, P. Eng, J. Stubbs, Y. Kono, and G. Shen, A Paris-Edinburgh cell for liquid silicate structural studies using monochromatic diffraction and soller slits, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Waszek, L., K. Arredondo, G. Finkelstein, L. Kellogg, L. Vadran, M. Li, C. Lithgow-Bertelloni, B. Romanowicz, N. Schmerr, M. Rudolph, J. Townsend, Z. Xing, and F. Yang, Slab stagnation in the lower mantle: A multidisciplinary investigation, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Wilson, R. and D. Cahill, Anisotropic deviations from Fourier's law in Si and MgO and the importance of temperature-profile extrema, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Wu, X., J. F. Lin, J. Liu, Z. Mao, X. Guo, C. McCammon, Y. Xiao, and V. Prakapenka, Elasticity of single-crystal phase D across the spin transitions of ferrous and feric iron in the lower mantle, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Wu, Y., X. Wu, J. F. Lin, T. Yoshino, C. McCammon, Y. Xiao, and V. Prakapenka, Electronic spin and valence states of iron in the Al-rich NAL and CF phases in the subducted slabs, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Xi, X., C. Ma, Z. Liu, Z. Chen, W. Ku, H. Berger, C. Martin, D. B. Tanner, and G. L. Carr, Probing the pressure-induced topological phase transition in BiTeI, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Ye, Y., C. Gu, S. H. Shim, V. Prakapenka, and Y. Meng, In situ measurements of the post-spinel and post-garnet phase boundaries in pyrolite at 17-32 GPa and 1500-2400 K, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Yoo, C. S., High energy density solids: Novel materials design and discovery at extreme conditions, *Materials Research Lecture, California Institute of Technology* (Pasadena, CA, October 1, 2014).

Yoo, C. S., Novel material design and discovery at extreme conditions, *Colloquium at the Department of Chemistry, Eastern Washington University* (Cheney, WA, November 6, 2014).

Yu, T., C. Prescher, J. Wang, V. Prakapenka, P. Eng, Y. Kono, J. Stubbs, and G. Shen, Structure study of sodium disilicate glass in a Paris-Edinburgh cell using monochromatic x-ray diffraction and a multi-channel collimator, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Zepeda-Alarcon, E., R. Lebensohn, P. Kaercher, and H. R. Wenk, Viscoplastic modeling of $MgSiO_3$ perovskite and periclase aggregates, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Zhang, L., Y. Meng, D. Popov, J. Wang, and H. K. Mao, Application of multigrain crystallography to mineralogy of the deep Earth, *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Zhang, L., Y. Meng, W. Yang, L. Wang, W. Mao, Q. Zeng, J. S. Jeong, A. J. Wagner, K. A. Mkhoyan, W. Liu, R. Xu, and H. K. Mao, Disproportionation of (Mg,Fe)SiO_3 perovskite and its implications to the deep earth (Invited), *Eos Trans. AGU Fall Meet., Suppl.* **95** (2014).

Zhang, P., R. E. Cohen, and K. Haule, Magnetic properties of FeO: a DFT+DMFT study, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Zhao, Z., S. Wang, A. Oganov, P. Chen, H. Zhang, Z. Liu, and W. Mao, Pressure-induced insulator to metal transitions in potential 3D topological insulators Ag_2Se and Ag_2Te, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Zhuravlev, K., A. F. Goncharov, S. Tkachev, P. Dera, and V. Prakapenka, P-V-T equation of state of SiC-3C: implications for primary pressure scale, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 3-7, 2014).

Zurek, E., Structure prediction from first principles (invited), *Texas Women's University* (Dallas, TX, March, 2014).

Zurek, E., Chemistry under pressure, *Department of Chemistry Seminar, University of Calgary* (Calgary, Canada, January, 2015).

4. References

1. Dzeiwonski, A. M. and D. L. Anderson, Preliminary reference Earth model, *Phys. Earth Planet. Inter* **25**, 297-356 (1981).
2. Yoder Jr., H. S., *Centenial History of the Carnegie Institution of Washington: The Geophysical Laboratory* (Cambridge University Press, New York, 2004).
3. Rhodes, R., *The Making of the Atomic Bomb* (Simon and Schuster, New York, 1986).
4. Mauger, L., M. S. Lucas, J. A. Munoz, S. J. Tracy, M. Kresch, Y. Xiao, P. Chow, and B. Fultz, Nonharmonic phonons in -iron at high temperatures, *Phys. Rev. B* **90**, 064303 (2015).
5. Körmann, F., B. Garbowski, B. Dutta, T. Hickel, L. Mauger, B. Fultz, and J. Neugebauer, Temperature dependent magnon-phonon coupling in bcc Fe from theory and experiment, *Phys. Rev. Lett.* **113**, 165503 (2014).
6. Smith, R. F., J. H. Eggert, R. Jeanloz, T. S. Duffy, D. G. Braun, J. R. Patterson, R. E. Rudd, J. Biener, A. E. Lazicki, A. V. Hamza, J. Wang, T. Braun, L. X. Benedict, P. M. Celliers, and G. W. Collins, Ramp compression of diamond to five terapascals, *Nature* **511**, 330-333 (2014).
7. Chen, B., Z. Li, D. Zhang, J. Liu, M. Y. Hu, J. Zhao, W. Bi, E. E. Alp, Y. Xiao, P. Chow, and J. Li, Hidden carbon in Earth's inner core revealed by shear softening in dense Fe_7C_3, *Proc. Nat. Acad. Sci.* **111**, 17755-17758 (2014).
8. Tomasino, D., M. Kim, J. Smith, and C. S. Yoo, Pressure-induced symmetry-lowering transition in dense nitrogen to layered polymeric nitrogen (LP-N) with oclossal Raman intensity, *Phys. Rev. Lett.* **113**, 205502 (2014).
9. Zha, C. S., R. E. Cohen, H. K. Mao, and R. J. Hemley, Raman measurements of phase transitions in dense solid hydrogen and deuterium to 325 GPa, *Proc. Nat. Acad. Sci.* **111**, 4792-4797 (2014).
10. Naumov, I. I. and R. J. Hemley, Aromacity, closed-shell effects, and metallization of hydrogen, *Acc. Chem. Res.*, dx.doi.org/10.1021/ar5002654 (2014).
11. Rozsa, V. F. and T. A. Strobel, Triple guest occupancy and negative compressibility in hydrogen-loaded b-hydroquinone clathrate, *J. Phys. Chem. Lett.* **5**, 1880-1884 (2014).
12. Schmandt, B., S. D. Jacobsen, T. W. Becker, Z. Liu, and K. G. Dueker, Dehydration melting at the top of the lower mantle, *Science* **344**, 1265-1268 (2014).
13. Water discovered deep beneath Earth's surface, http://www.usatoday.com/story/news/nation/2014/2006/2012/water-earth-reservoir-science-geology-magma-mantle/10368943/ (2014).
14. Smith, S. J., M. M. Bishop, J. M. Montgomery, T. P. Hamilton, and Y. K. Vohra, Polymorphism in paracetamol: Evidence of additional forms IV and V at high pressure, *J. Phys. Chem. A* **118**, 6068-6077 (2014).
15. Boulard, E., D. Pan, G. Galli, Z. Liu, and W. L. Mao, Tetrahedrally coordinated carbonates in Earth's lower mantle, *Nature Comm.* **6**, 6311 (2015).
16. Zhao, Z., E. F. Wang, H. Yan, Y. Kono, B. WEn, L. Bai, F. Shi, J. Zhang, C. Kenney-Benson, C. Park, Y. Wang, and G. Shen, Nanoarchitectured materials composed of fullerene-like spheroids and disordered graphene layers with tunable mechanical properties, *Nature Comm.* **6**, 6212 (2015).
17. Lipp, M. J., Z. Jenei, D. Ruddle, C. Aracne-Ruddle, H. Cynn, W. J. Evans, Y. Kono, C. Kenney-Benson, and C. Park, Equation of state measurements by radiography provide evidence for a liquid-liquid phase transition in cerium, *J. Phys.: Conf. Series* **500**, 032011 (2014).
18. Doherty, M. W., V. V. Struzhkin, D. A. Simpson, L. P. McGuinness, Y. Meng, A. Stacey, T. J. Karle, R. J. Hemley, N. B. Manson, L. C. L. Hollenberg, and S. Prawer, Electronic properties and metrology of the diamond NV- center under pressure, *Phys. Rev. Lett.* **112**, 047601 (2014).