APS March Meeting 2011
Dallas, Texas
http://www.aps.org/meetings/march/index.cfm
Tuesday, March 22, 2011 8:00AM - 10:48AM —
Session H31 DMP GSCCM DCOMP: Focus Session: Materials at High Pressure I: Molecular and Simple Materials C145

8:00AM H31.00001 Structural investigation and shock Hugoniots calculations of methane under high temperatures and pressures BENJAMIN SHERMAN, California State University, Northridge, BURKHARD MILITZER, HUGH WILSON, University of California, Berkeley, DAYANTHIE WEERARATNE, California State University, Northridge — The behavior of methane under pressures and temperatures spanning 0.02-7.75 Mbar and 300-300,000 K was studied using density functional molecular dynamics. The structural properties of fluid and crystalline methane were analyzed with simulations at various (P,T) conditions. These simulations were also used to calculate the shock Hugoniot curves of methane for a range of initial densities between 0.4-0.57 g/cc. These curves allow us to make predictions of state and phase that correspond to future methane shock experiments.

8:12AM H31.00002 Proton Exchange Reactions in Deuterium Water Mixtures¹, GUSTAV BORSTAD, Institute for Shock Physics, Dept. of Physics, Washington State University, Pullman, WA 99164, CHOONG-SHIK YOO, Institute for Shock Physics, Dept. of Chemistry, Washington State University, Pullman, WA 99164 — Binary mixtures of water and hydrogen under pressure are of interest both as fundamental systems in physics and chemistry and due to their applicability to fuel cells. Their behaviors at extreme pressures and temperatures are also of significance to understanding the interaction of chemical species in the interiors of giant gas planets and other planetary objects. In this talk, we will present high-pressure Raman data of deuterium water mixtures, which provides both kinetic information regarding the proton exchange reactions and the structure of deuterium in the mixtures.

³The work has been supported by NSF (DMR-0854618) and DOE-NNSA (# DE-F6003-97SF21388).

8:24AM H31.00003 Zero-Temperature Structures of Atomic Metallic Hydrogen, JEFFREY MCMAHON, DAVID CEPERLEY, Department of Physics, University of Illinois, Urbana-Champaign, IL 61801 — Since the first prediction of an atomic metallic phase of hydrogen by Wigner and Huntington over 75 years ago, there have been many theoretical efforts aimed at determining the crystal structures of the zero-temperature phases. We present results from ab initio random structure searching with density functional theory performed to determine the ground state structures from 500 GPa to 5 TPa. We estimate that molecular hydrogen dissociates into a monatomic body-centered tetragonal structure near 500 GPa ($r_s = 1.225$), which then remains stable to 2.5 TPa ($r_s = 0.969$). At higher pressures, hydrogen stabilizes in an ...ABCABC... planar structure that is remarkably similar to the ground state of lithium, which compresses to the face-centered cubic lattice beyond 5 TPa ($r_s < 0.80$). Our results provide a complete ab initio description of the atomic metallic crystal structures of hydrogen, resolving one of the most fundamental and long outstanding issues concerning the structures of the elements.

8:36AM H31.00004 Phase Diagram of Carbon Dioxide at High Pressure and Temperatures: Implications to the Deep Carbon Cycle¹, CHOOENG-SHIK YOO, Dept of Chemistry and Institute for Shock Physics, Washington State University, Pullman, WA 99164, AMARTYA SENGUPTA, Institute for Shock Physics, Washington State University, Pullman, WA 99164 — Carbon dioxide is an important terrestrial volatile often considered to exist in the deep interior of the Earth. The phase diagram of carbon dioxide is critical to validate such hypothesis. In this study, we will present the phase diagram of carbon dioxide including the most recent finding of coesite-like carbon dioxide, a missing analog to SiO$_2$, address several controversies in terms of phase metastabilities and thermal path dependent transitions, and discuss about the implication to the deep carbon cycle.

³The work has been supported by NSF (DMR-0854618) and DARPA (W911NF-10-1-0081).

8:48AM H31.00005 Structural and optical properties of liquid CO$_2$ up to 1 terapascal¹, BRIAN BOATES, Lawrence Livermore National Laboratory & Dalhousie University, SEBASTIEN HAMEL, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, STANIMIR BONEV, Lawrence Livermore National Laboratory & Dalhousie University — The properties of liquid CO$_2$ have been studied through first-principles molecular dynamics simulations in the pressure-temperature range of 0-1 TPa and 200-100,000 K. The resulting equation of state data is used to predict shock Hugoniots for several initial conditions. Comparison with available experimental data up to 70 GPa is excellent. We find a gradual phase transition characterized by the destabilization of CO$_2$ molecules and the formation of other molecular compounds. The liquid phase diagram is divided into several regimes based on a thorough analysis on changes in bonding, structural properties, and chemical composition. Calculations of optical properties such as conductivity and reflectivity will also be discussed.

¹Work supported by NSERC, LLNL, the Killam Trusts, and Acenet. Prepared by LLNL under Contract DE-AC52-07NA27344.

9:00AM H31.00006 Density Functional Theory (DFT) simulations of CO2 under shock compression and design of liquid CO2 experiments on Z¹, T. R. MATTSSON, L. SHULENBURGER, S. ROOT, Sandia National Laboratories, Albuquerque, NM., K. R. COCHRANE, Ktech Corporation, Albuquerque, NM. — Quantitative knowledge of the thermo-physical properties of CO2 at high pressure is required to confidently model the structure of gas-giants like Neptune and Uranus and the deep carbon cycle of the earth. DFT based molecular dynamics has been established as a method capable of yielding high fidelity results for many materials, including shocked gases, at high pressure and temperature. We predict the principal Hugoniot for liquid CO2 up to 500GPa. Our simulations also show that the plateau in shock pressure identified by Nellis and co-workers [1] is the result of dissociation. At low temperatures we validate the DFT results by comparing with diffusion Monte Carlo calculations. This allows for a more accurate determination of the initial conditions for the shock experiments. We also describe the design of upcoming flyer-plate experiments on the Z-machine aimed at providing high-precision shock compression data for CO2 between 150 and 600 GPa. [1] W. Nellis, et. al. , J. Chem. Phys. 95, 5268 (1991).

¹Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corp. for the US Dept. of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL85000.

9:12AM H31.00007 Novel phases of simple substances at megabar pressures, MIKHAIL EREMETS, Max Planck Institute for Chemistry — Under megabar pressures solids can be strongly compressed: volume of solid hydrogen decreases in ~20 times, even diamond is 1.5 fold compressed at achievable pressures of ~300 GPa. This dramatically changes interatomic distances in materials eventually leading to metallization in a number of presenting substances. Metals under compression supposedly remain in metallic state. But at high densities the core electrons come in to play and the electronic structure significantly departs from the simple metal as it was demonstrated for lithium. We present an ultimate case: sodium - simple metal - becomes transparent at pressures of ~200 GPa transforming into ionic- electrode-like state. We will present also our recent studies on nitrogen and nitrogen-rich materials: ammonia, azides and others, and progress on studies at pressures ~400 GPa.
However, because diamond is difficult to deform, little is known with regard to its constitutive properties such as yield strength. In this work, we present results from ab initio calculations. The same DAC experiment. Calibration curve of the Raman shift vs plastic flow of diamond at total strains of 10% and 5%, respectively, indicating that diamond weakens rapidly when temperature is over 1000 °C. We further derived the micro stress of diamond from peak width analysis, and found that the micro and macro stresses show similar variations with total strain at both room temperature and 1000 °C. However, at 1200 °C, the micro stress remains constant in entire deformation, indicating that stress is uniformly distributed within diamond particles at 1200 °C. We also carried out SEM studies on the recovered samples to investigate the microstructures, and find that the grain size of diamond decreases substantially during the deformation, from the initial microns to sub-microns for the room temperature deformation, however, almost doesn’t change for the 1200 °C.

10:12AM H31.00010 New primary pressure calibrants for high pressure and temperature scale: SiC-3C and cBN are possible candidates, KIRILL ZHURAVLEV, ALEXANDER GONCHAROV, Carnegie Institution of Washington, VITALI PRAKAPENKA, University of Chicago — Since the invention of a diamond-anvil cell, various high-pressure scales for in situ pressure measurements have been realized. Ruby-based pressure scale (Mao et al., 1986) is the best known and high-pressure scientific community has been using it for over two decades. However, it has limited use at elevated temperatures, due to the weakening and broadening of the ruby fluorescence line. The recent developments in the field of high temperature, high pressure physics and geophysics require some alternative pressure scale, capable of measuring pressures at temperatures up to 3000 K. Cubic boron nitride (cBN) was recently proposed as the possible pressure calibrant. It has been suggested that the simultaneous use of x-ray diffraction to measure density and Brillouin spectroscopy to obtain elastic properties of the crystal can be used to construct the pressure scale independent of any other pressure standards. However, the acoustic velocities of cBN are very close to those of diamond and, therefore, are hard to resolve in experiment in diamond-anvil cell. Another possible primary pressure calibrant is cubic silicon carbide (SiC-3C). We performed single crystal x-ray diffraction and Brillouin spectroscopy up to 1 Mbar in pressure at room temperature in the diamond-anvil cell and show that cBN and SiC-3C, indeed, can be used in constructing reliable and accurate high-pressure, high-temperature scale.

10:24AM H31.00011 Formation and superconductivity of hydrides under pressure1, DUCK YOUNG KIM, TCM group, Cavendish laboratory, University of Cambridge, UK, RALPH H. SCHEICHER, Uppsala University, Sweden, CHRIS J. PICKARD, University College London, UK, RICHARD J. NEEDS, TCM group, Cavendish laboratory, University of Cambridge, UK, RAJEEV AHUJA, Uppsala University, Sweden — Hydrogen is the lightest and smallest element in the periodic table. Despite its simplest electronic structure, enormous complexity can arise when hydrogen participates in the formation of solids. Pressure as a controllable parameter can provide an excellent platform to investigate novel physics of hydrides because it can induce structural transitions and even changes in stoichiometry accompanied with phenomena such as metallization and superconductivity. In this presentation, we will briefly overview contemporary high-pressure research on hydrides and show our most recent results on predicting crystal structures of metal hydrides under pressure using ab initio random structure searching. Our findings allow for a better understanding of pressure-induced metallization/superconductivity in hydrides which can help to shed light on recent observations of pressure-induced metallization and superconductivity in hydrogen-rich materials.

1Membership pending


9:48AM H31.00008 Diamond as a high pressure gauge up to 2.7 MBar, NATALIA DUBROVINSKAIA, LEONID DUBROVINSKY, RAZVAN CARACAS, MICHAEL HANFLAND — Diamond anvil cell (DAC) technique has become a very important method of probing materials behaviour under pressure in various fields of research ranging from physics to biology and geosciences. Optical methods of pressure determining in DAC experiments are based on fluorescent markers or calibrated pressure dependence of the Raman shift of suitable materials. Diamond has been since long recognised as a good pressure marker in experiments conducted in a diamond anvil cell. It is stable at ultra-high pressures that allows one to use the pressure dependence of the Raman frequency of the LTO optical phonon of diamond as a pressure gauge. A pressure gauge is a key issue of any high pressure experiment in a diamond anvil cell. Here we present a method of in situ synthesis of microcrystals of diamond that can be further used as a pressure standard in course of the same DAC experiment. Calibration curve of the Raman shift vs pressure is extended up to 270 GPa and experimental results are compared with those of ab initio calculations.

10:00AM H31.00009 High-pressure and high temperature deformation studies of polycrystalline diamond, XIAOHUI YU — With Vicker’s hardness 120 GPa, shear modulus 535 GPa, diamond is the hardest material known to mankind. However, because diamond is difficult to deform, little is known with regard to its constitutive properties such as yield strength. In this work, we present results obtained at NSLS using deformation-DIA on polycrystalline diamond at different P-T conditions. As expected, even at total strains up to 20%, we did not observe the yield point of diamond at room temperature and a confining pressure of 4 GPa. However, for deformation at 1000 and 1200 °C, we observed an plastic flow of diamond at total strains of 10% and 5%, respectively, indicating that diamond weakens rapidly when temperature is over 1000 °C. We further derived the micro stress of diamond from peak width analysis, and found that the micro and macro stresses show similar variations with total strain at both room temperature and 1000 °C. However, at 1200 °C, the micro stress remains constant in entire deformation, indicating that stress is uniformly distributed within diamond particles at 1200 °C. We also carried out SEM studies on the recovered samples to investigate the microstructures, and find that the grain size of diamond decreases substantially during the deformation, from the initial microns to sub-microns for the room temperature deformation, however, almost doesn’t change for the 1200 °C.

10:12AM H31.00010 New primary pressure calibrants for high pressure and temperature scale: SiC-3C and cBN are possible candidates, KIRILL ZHURAVLEV, ALEXANDER GONCHAROV, Carnegie Institution of Washington, VITALI PRAKAPENKA, University of Chicago — Since the invention of a diamond-anvil cell, various high-pressure scales for in situ pressure measurements have been realized. Ruby-based pressure scale (Mao et al., 1986) is the best known and high-pressure scientific community has been using it for over two decades. However, it has limited use at elevated temperatures, due to the weakening and broadening of the ruby fluorescence line. The recent developments in the field of high temperature, high pressure physics and geophysics require some alternative pressure scale, capable of measuring pressures at temperatures up to 3000 K. Cubic boron nitride (cBN) was recently proposed as the possible pressure calibrant. It has been suggested that the simultaneous use of x-ray diffraction to measure density and Brillouin spectroscopy to obtain elastic properties of the crystal can be used to construct the pressure scale independent of any other pressure standards. However, the acoustic velocities of cBN are very close to those of diamond and, therefore, are hard to resolve in experiment in diamond-anvil cell. Another possible primary pressure calibrant is cubic silicon carbide (SiC-3C). We performed single crystal x-ray diffraction and Brillouin spectroscopy up to 1 Mbar in pressure at room temperature in the diamond-anvil cell and show that cBN and SiC-3C, indeed, can be used in constructing reliable and accurate high-pressure, high-temperature scale.

10:24AM H31.00011 Formation and superconductivity of hydrides under pressure, DUCK YOUNG KIM, TCM group, Cavendish laboratory, University of Cambridge, UK, RALPH H. SCHEICHER, Uppsala University, Sweden, CHRIS J. PICKARD, University College London, UK, RICHARD J. NEEDS, TCM group, Cavendish laboratory, University of Cambridge, UK, RAJEEV AHUJA, Uppsala University, Sweden — Hydrogen is the lightest and smallest element in the periodic table. Despite its simplest electronic structure, enormous complexity can arise when hydrogen participates in the formation of solids. Pressure as a controllable parameter can provide an excellent platform to investigate novel physics of hydrides because it can induce structural transitions and even changes in stoichiometry accompanied with phenomena such as metallization and superconductivity. In this presentation, we will briefly overview contemporary high-pressure research on hydrides and show our most recent results on predicting crystal structures of metal hydrides under pressure using ab initio random structure searching. Our findings allow for a better understanding of pressure-induced metallization/superconductivity in hydrides which can help to shed light on recent observations of pressure-induced metallization and superconductivity in hydrogen-rich materials.

1Membership pending
11:15AM J31.00001 Multi-Scale Shock Compression Simulations of Metals and Metallic Phase Transitions1. N. GOLDMAN, LARRY FRIED, Lawrence Livermore National Laboratory — We present a straightforward method for efficient molecular dynamics (MD) simulation of shock compression of materials that experience thermal electronic excitations at high pressure and temperature. Previous studies have shown that exclusion of the electronic temperature at extreme conditions can result in incorrect computation of dynamic and equation of state properties. The Multi-Scale Shock Technique (MSST) is a simulation methodology based on the Navier–Stokes equations for compressible flow that enables MD simulation of a shock wave with relatively small computational cost. We extend MSST to allow for changes in the electronic entropy during shock compression while conserving Hugoniot conditions. This allows for simulation of significantly higher shock velocities than previously possible with MSST. We have used our simulation methodology in density functional tight binding simulations of shock compressed silicon. We observe that at high shock velocities inclusion of a non-zero electron temperature results in lower computed shock Hugoniot temperatures and pressures. Our methodology is well suited for shock compression simulations of any material that experiences changes in its electronic entropy under extreme thermodynamic conditions.

1Prepared by LLNL under Contract DE-AC52-07NA27344.

11:27AM J31.00002 Large-Scale Molecular Dynamics Simulations of Shock-Induced Plasticity in Tantalum Single Crystals1. R. RAVELO2, University of Texas-El Paso, QI AN, California Institute of Technology, T.C. GERMANN, B.L. HOLIAN, Los Alamos National Laboratory — We report on large-scale non-equilibrium molecular dynamics (NEMD) simulations of shock wave compression in Ta single crystals. The atomic interactions are modeled via a recently developed and optimized embedded-atom method (EAM) potential for Ta, which reproduces the equation of state up to 200 GPa. We examined the elastic-plastic transition and shock wave structure for wave propagation along the low index directions: (100), (110) and (111). Shock waves along (100) and (111) exhibit an elastic precursor followed by a plastic wave for particle velocities below 1.1 km/s for (100) and 1.4 km/s for (111). The nature of the plastic deformation along (110) is dominated by twinning for pressures above 40 GPa.

1Part of this work was supported by the U.S. Department of Energy under contract DE-AC5206NA25396.
2Computational Physics Division, Los Alamos National Laboratory

11:39AM J31.00003 Transport of particulate matter from a shocked interface1. W.T. BUTTLER, J.E. HAMMERBERG, D. ORO, C. MORRIS, F. MARÍA, C. ROUSCULP, Los Alamos National Laboratory — We have performed a series of shock experiments to measure the evolution and transport of micron and sub-micron Tungsten particles from a 40 micron thick layer deposited on an Aluminum substrate. Densities and velocity distributions were measured using proton radiography at the Los Alamos Neutron Science Center for vacuum conditions and with contained Argon and Xenon gas atmospheres at initial pressures of 9.5 bar and room temperature. A common shock drive resulted in free surface velocities of 1.25 km/s. An analysis of the time dependence of Lithium Niobate piezo-electric pin pressure profiles is given in terms of solutions to the particulate drag equations and the evolution equation for the particulate distribution function. The spatial and temporal fore-shortening in the shocked gas can be accounted for using reasonable values for the compressed gas shear viscosities and the vacuum distributions. The detailed form of the pin pressure data for Xenon indicates particulate breakup in the hot compressed gas.

1This work supported by the U.S. Department of Energy under contract DE-AC52-06NA25396.

11:51AM J31.00004 Thermal Emission Determination of Argon under Extreme Pressure and Temperature. D. ALLEN DALTON, MICHAEL WONG, ALEXANDER F. GONCHAROV, JULIUS OJWANG, VIKTOR V. STRUZHKN. Geophysical Laboratory, Carnegie Institution of Washington, ZUZANA KONOPKOVA, PETER LAZOR, Department of Earth Sciences, Uppsala University — Argon is a common pressure-transmitting medium in diamond anvil cell (DAC) experiments, and is often used as thermal insulation in the laser heated DAC. A more thorough understanding of the thermal properties of argon under extreme conditions is essential for measuring thermal properties of materials under similar conditions. A transient heating technique was applied to a symmetric DAC up to 50 GPa and 2500 K. A 1 μm thick iridium foil positioned within a recessed gasket hole filled with argon served as a laser absorber to pump thermal energy into the sample. Pump pulses of 6 μs temporal width were provided from an electronically modulated Yb-based fiber laser. We determined the temperature of the coupler with 500 ns time resolution by applying a Planckian fit to the thermal emission spectrum. Finite element calculations were also used to simulate thermal diffusion in the DAC cavity. The experimental results show slightly larger thermal conductivity with theory, but the results converge in the limit of high temperature. This work is supported by NSF EAR 1015239, NSF-REU, Carnegie Institution of Washington, and DOE-NNSA (CDAC).

12:03PM J31.00005 Thermal diffusivity of metals at high pressure1. BRUCE BAER, WILLIAM EVANS, Lawrence Livermore National Laboratory — Very few measurements of thermal diffusivity have been taken at high pressure. This is especially true of metals above 2 GPa. In earlier experiments, the Angstrom method has been employed for these types of measurements. However, this method is limited for high pressure because it requires a relatively large sample. We will discuss the use of sinusoidally modulated laser heating to measure thermal diffusivity in the diamond-anvil-cell.

1This work was performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344.

12:15PM J31.00006 Pressure-Induced Structure Transitions in Europium Metal to 92 GPa1. W. BI, J. SCHILLING, Department of Physics, Washington University in Saint Louis, Y. MENG, HPCAT, Carnegie Institution of Washington, Argonne National Laboratory, R. KUMAR, A. CORNELIUS, Y. ZHANG, C. CHEN, HPCSEC and Department of Physics, University of Nevada, Las Vegas, R. HENNIG, Department of Materials Science and Engineering, Cornell University — Motivated by the recent discovery of pressure-induced superconductivity in Eu for pressures above 80 GPa [1], we have carried out high pressure angle-dispersive synchrotron x-ray diffraction measurements on Eu metal in a diamond anvil cell to 92 GPa. Our experiments confirm the bcc-to-hcp transition at 12 GPa reported in previous studies and identify two further phase transitions. The predictions of two independent density functional theory calculations are compared to the experimental results.


1This research is supported by NSF grant DMR-0703896 and by the Carnegie/DOE Alliance Center (CDAC) through NNSA/DOE grant number DE-FC52-08NA28554.
**12:27PM J31.00007 Electronic structure and dynamics of elements at high pressures**

MAO, Carnegie Institution of Washington — Electronic structure and dynamics information of materials under high pressure has been very scarce due to the experimental difficulties. The standard electronic probes using electron energy loss spectroscopy (EELS) is limited to vacuum pressures. The optical probes that can reach high-pressure samples through the diamond windows, on the other hand, are limited by the energy accessibility (<5 eV) and near-zero momentum transfer, \( q = (\Delta q/\lambda_0) \sin \theta \). These problems can be overcome by the newly advanced, two-photon, inelastic, x-ray, scattering (IXS) spectroscopy which uses high energy x-rays (\( \sim 10^4 \) eV) to provide the atomic-level momentum transfer and to enter (with energy \( E \)) and exit (with energy \( E_0 \)) the pressure vessel. The electronic spectra are revealed by analyzing the x-ray energy loss between the two photons, \( h\omega = E - E_0 \). Using IXS facilities at third-generation synchrotron source, we studied electronic structure and dynamics of two elements at high pressures in a diamond anvil cell: i.e., He, the widest-gap insulator, and Na, the archetypal free-electron metal. At 11.9-17.9 GPa in a single crystal, we observed rich electron excitation spectra, including a cut-off edge above 23 eV, a sharp exciton peak showing linear volume dependence, and a series of excitations and continuum at 26 to 45 eV. We determined electronic dispersion along the 100 direction over two Brillouin zones, and provided a quantitative picture of the helium exciton beyond the simplified Wannier-Frenkel description. At 1.6-4.39 GPa in a polycrystalline Na sample, we observed the sharp plasmal peak at low \( q \) and its dispersion beyond the critical \( q_c \). The plasmon shifts to higher energy under compression and drastic reduction of \( r_s \). 

**1:03PM J31.00008 Diffusion Monte Carlo calculations of Xenon melting under pressure**

SHULENBURGER, T.R. MATTSSON, Sandia National Laboratories — The slope of the melting temperature as a function of pressure yields, via the Clausius-Clapeyron equation, important information regarding the changes in density, energy, and entropy. It is therefore crucial to resolve the long-standing differences in melt lines under pressure between Diamond Anvil Cell data (low/flat melt line) and other methods, including density functional theory (DFT) simulations (high/steep melt line). The disagreement for Ta was recently resolved and although a similar situation exists in the literature on Xe, the resolution may be quite different. DFT with its lack of van der Waals forces is a prima facie less credible simulation method for Xe, although excellent agreement has been obtained between calculations of the Hugoniot of Xe and experiments. We investigate whether this theoretical shortcoming is significant for the melting transition by applying diffusion Monte Carlo. The energy differences obtained in this way are compared to the DFT results in order to address any systematic errors that may be present near the melting transition.

**1:15PM J31.00009 Lattice dynamics at ultra-high pressures using high-resolution inelastic x-ray scattering**

FARBER, Lawrence Livermore National Laboratory — While our understanding of many physical properties is enhanced by the large body of neutron, the restrictions on sample size imposed by the technique relegated the achievable information to low or at most, moderate pressures (\( \sim 10 \) GPa) and to materials readily available in reasonable large quantities. The advent of third generation synchrotron sources and the construction of beamlines dedicated for inelastic x-ray scattering experiments (IXS), these limitations have to a great degree been overcome. Over the past few years our group has focused a large experimental and theoretical effort on quantifying the vibrational energies in metals at high-pressures and high-temperatures. Most recently, we have determined the phonon dispersions across the isostructural gamma- to alpha-cerium transition. Our new data place important thermodynamical and theoretical constraints on the underlying physics of this important transition.

**1:27PM J31.00010 High-pressure phases of calcium**

TEWELDEBERHAN, JONATHAN DOBOIS, Lawrence Livermore National Laboratory, STANIMIR BONEV, Lawrence Livermore National Laboratory and Dalhousie University — The high-pressure phases of calcium have been investigated using a combination of density functional theory and diffusion quantum Monte Carlo calculations. Finite-temperature Gibbs free energies of several competing structures are computed at pressures near 50 GPa. The discrepancy between theory and experiment both at low and room temperature is resolved with input from diffusion quantum Monte Carlo. Furthermore, diffusion quantum Monte Carlo calculations are performed on 0 K crystalline structures up to 150 GPa. The resulting structures differ from those obtained with density functional theory.

**1:39PM J31.00011 Lifshitz transition in c16 Li at high pressures: Unfolding first-principles Fermi surfaces**

LIN, TOM BERLIJN, WEI KU, Brookhaven National Laboratory/ Stony Brook University — The Fermi surface topology of c16 Li is investigated using the recently developed first-principles band structure unfolding method [1]. The resulting unfolded Fermi surfaces display a clear Lifshitz transition at 47 GPa, explaining the anomalous change of superconducting transition temperature [2]. The unfolded Fermi surfaces also reveal a more complete picture of the driving force of the c16 phase starting at 39 GPa [3]. In addition to the previously proposed “nesting” effect [3] along \( [\frac{1}{2} \frac{1}{2} 0] \), both \( [0 0 1] \) and \( [\frac{1}{2} \frac{1}{2} 0] \) wavevectors are found to contribute significantly to the structural instability as well, due to their large phase space, a more effective effect in 3D. We expect a wide rate of applications of this Fermi surface unfolding method to the study of high pressure electronic structure.

**1:51PM J31.00012 On the role of quantum ion dynamics for the anomalously melting of lithium**

SABRI ELATRESH, Department of Physics, Dalhousie University, Halifax, NS, B3H 3J5, Canada. STANIMIR BONEV, Lawrence Livermore National Laboratory, Livermore, California 94550 — Lithium has attracted a lot of interest in relation to a number of counterintuitive electronic and structural changes that it exhibits under pressure. One of the most remarkable properties of dense lithium is its anomalous melting. This behavior was first predicted theoretically based on first-principles molecular dynamics (FPMD) simulations, which treated the ions classically [1]. The lowest melting temperature was determined to be about 275 K at 65 GPa. Recent experiments measured a melting temperature about 100 K lower at the same pressure. In this talk, we will present FPMD calculations of solid and liquid lithium free energies up to 100 GPa that take into account quantum ion dynamics. We examine the significance of the quantum effects for the finite-temperature phase boundaries of lithium and, in particular, its melting curve.

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1. Work supported by LLNL, ACEnet, NSERC, and CFI. Prepared by LLNL under Contract DE-AC52-07NA27344.
2. Work supported by NSERC, Acenet, and LLNL under Contract DE-AC52-07NA27344.
3. The speaker would like to acknowledge collaborating researchers: R. Ahuja, Y. Cai, P. Chow, Y. Ding, P. Eng, R.J. Hemley, C.C. Kao, S. Lebegue, W.L. Mao, E.L. Shirley, J. Shu, & Y. Xiao.
2:03PM L31.00013 Graphite under high pressure, YUEJIAN WANG, Yale University — As one of the longest-known forms of carbon, graphite has been extensively studied for several decades. However, its phase diagram under high pressures is still poorly understood. Here we use both in-situ high-pressure Raman spectroscopy and synchrotron x-ray diffraction, collected on both compression and decompression, to elucidate the high-pressure behavior of highly-ordered pyrolytic graphite (HOPG) at room temperature. The Raman spectra show that G band (1580 cm$^{-1}$) at ambient pressure of HOPG shifts to higher frequency with increased pressure, which has been attributed to pressure-induced in-plane lattice contraction. Above 19 GPa the broadening of this Raman peak indicates a reordering of the atomic structure, and is consistent with synchrotron x-ray diffraction measurements that also show a slight change in symmetry.

Tuesday, March 22, 2011 2:30PM - 5:30PM –
Session L31 DMP GSCCM DCOMP: Focus Session: Materials at High Pressure III: Electronic Transitions C145

2:30PM L31.00001 Pressure Induced Metal Insulator Phase Transition in Eu$_2$Ir$_2$O$_7$, FAZEL FALLAH TAFTI, JUN ISHIKAWA, YO MACHIDA, ALIX MCCOLLAM, SATORU NAKATSUJI, STEPHEN JULIAN — The metal to insulator phase transition of the pyrochlore iridate Eu$_2$Ir$_2$O$_7$ has been studied by means of resistivity measurements under pressure in the range 2 to 12 GPa. At ambient pressure, the system is a “metal” at high temperatures with a non-metallic rise of resistivity with decreasing temperature followed by a metal-insulator phase transition at T$_{MI}$ below which it becomes insulating. With increasing pressure, a cross-over from non-metallic to metallic appears in the resistivity curves at a temperature T* > T$_{MI}$. As the pressure is further increased T* rises, T$_{MI}$ drops and the low temperature insulating phase melts into a metallic phase through a continuous transition at P $\sim$ 7.8 GPa. The high pressure metallic phase is rather curious and exhibits two characteristic features of Kondo metals: a minimum resistivity and a logarithmic rise of resistivity at low temperatures. We will show that there is a remarkable correspondence between the resistivity curves measured at various pressures and those obtained by successively replacing the R site of the R$_2$Ir$_2$O$_7$ family by larger rare earth atoms.

2:42PM L31.00002 Pressure-induced Metallization of Carbon Disulfide$^1$, RANGANATH DIAS, Institute for Shock Physic, Dept. of Physics, Washington State University, Pullman, WA 99164, MATHEW DEBESSAI, Institute for Shock Physic, Washington State University, Pullman, WA 99164, CHOONG-SHIK YOO, Institute for Shock Physics, Dept. of Chemistry, Washington State University, Pullman, WA 99164. — We will report high pressure electrical resistivity measurements on solid CS$_2$ in diamond anvil cell to 60GPa. The result shows a steady decrease in resistivity to that of metal at around 55GPa. Its visual appearance of CS$_2$ also supports its insulator-metal transition: the initially transparent CS$_2$ becomes opaque and eventually reflective with increasing pressure. We will also present a plausible mechanism for the observed metallization.

$^1$The work has been supported by NSF (DMR-0854618) and DTRA (HDTTRA1-09-1-0041).

2:54PM L31.00003 Electrical resistance measurement of optimal doped YBCO under pressure, TAKAKI MURAMATSU, TsSUH, University of Houston, DUC PHAM TEAM, CHING-WU CHU TEAM — High pressure effect on nearly optimal doped high T$_C$ cuprate superconductor YBa$_2$Cu$_3$O$_{7-x}$ was studied by the electrical resistance measurements up to about 30 GPa. Superconducting phase of YBa$_2$Cu$_3$O$_{7-x}$ in pressure-temperature phase diagram was confirmed. T$_C$ has the broad maximum at about 8 GPa and then decreases with pressure and disappears at the pressure between 23 GPa and 25 GPa. In higher pressure region, the resistance shows upturn below about 60 K, indicating the possibility of crossover on YBa$_2$Cu$_3$O$_{7-x}$ from superconductor to semiconductor at about 24 GPa

3:06PM L31.00004 Pressure induced phase transition in FeGa alloys, CHRISTOPHER DEVREUGD, Virginia Tech University, MUHTAR AHART, Carnegie Institution of Washington, PETER GEHRING, NIST Center for Neutron Research, DWIGHT VIEHLAND, Carnegie Virginia Tech University, RUSSELL HEMLEY, Carnegie Institution of Washington — Giant magnetostriction in Fe–x Ga alloys (15–x - 27) offers potential for future generations of sensors and actuators. A maximum in the magnetostrictive strain is found at Ga content of about 19 percent, which is ten times higher than that of pure alpha-Fe. To investigate the behavior of FeGa alloys under pressure, we chose a slow cooled alloy of FeGa-19 as our sample and performed x-ray diffraction experiments in a diamond anvil cell up to 45 GPa. Diffraction pattern shows powder rings associated with (110), (200), and (211) Bragg reflections from expected bcc structure of iron below 24 GPa. We also observed the intensity increases along the powder rings associated with the crystal structure of Galfenol. Considering the (110) Bragg peak splits into three peaks above 24 GPa, our results indicate that FeGa alloy undergoes a bcc cubic to a hexagonal transition around 24 GPa. When the pressure is decreased, the hcp phase transforms back to the bcc phase. The transition mechanism can be understood by using the analogy to the bcc-hcp phase transition in pure iron under pressure. The transition in iron is a martensitic or displacive one. The hcp structure can be derived from the bcc structure through a relatively minor distortion of the bcc structure.

3:18PM L31.00005 High Pressure Studies of UO$_2$$_3^1$, ZSOLT JENEI, MAGNUS LIPP, JAE-HYUN KLEPEIS, BRUCE BAER, HYUNCHAE CYNN, WILLIAM EVANS, Lawrence Livermore National Laboratory, CHANGYONG PARK, DIMITRI POPOV, HPCAT, Advanced Photon Source, Argonne National Laboratory — It has been reported that upon compression at ambient temperature δ-UO$_2$ becomes amorphous at 2.2 GPa. (Journal of Alloys and Compounds 315 p59-61). We studied the properties of γ-UO$_3$ in diamond anvil cell up to 75 GPa. Powder diffraction experiments performed at HPCAT/Advanced Photon Source show the crystalline uranium trioxide transforms to an amorphous solid between 12 and 14 GPa and remains amorphous up to 75 GPa. The transition has been confirmed by Raman spectroscopy as well. In this paper we’ll present our findings on the amorphous transition together with the equation of state of both the crystalline phase and the amorphous phase.

$^1$This work performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344. HPCAT is supported by CIW, CDAC, UNLV and LLNL through funding from DOE-NNSA, DOE-BES and NSF. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH11357.

3:30PM L31.00006 High-pressure equation of state of U$_3$O$_8$, JAE-HYUN KLEPEIS, ZSOLT JENEI, MAGNUS LIPP, WILLIAM EVANS, Lawrence Livermore National Laboratory, DIMITRI POPOV, HPCAT, APS, Argonne National Laboratory, CHANGYONG PARK, HPCAT APS Argonne National Laboratory — We will present experimental studies at high pressures of the equation of state of U$_3$O$_8$. Isothermal pressure-volume measurements of U$_3$O$_8$ were made at ambient/elevated (600 K) temperatures in the pressure range of 1 atm ~ 80 GPa (10 ~ 70 GPa). Angle dispersive x-ray diffraction patterns at ambient temperature indicate that the A-centered orthorhombic structure of U$_3$O$_8$ transforms to the face centered cubic (fcc) structure above 9 GPa. Both the orthorhombic and cubic phases co-exist between 9 GPa and 30 GPa. As the temperature is increased at 10 GPa, we find that U$_3$O$_8$ also transforms to the fcc structure. As the pressure is increased at 600 K, the fcc structure undergoes a phase transition to the body centered tetragonal structure. Since the uranium in U$_3$O$_8$ is the dominant x-ray scatterer, the behavior of the oxygen at the phase transitions was measured using Raman spectroscopy.

$^1$This work was performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344. HPCAT is supported by CIW, CDAC, UNLV and LLNL through DOE-NNSA, DOE-BES and NSF. APS is supported by DOE-BES, under Contract DE-AC02-06CH11357.
3:42PM L31.00007 High pressure x-ray diffraction of uranium oxide formed by natural oxidation of uranium, HYUNCHAE CYNN, WILLIAM J. EVANS, BRUCE J. BAER, Lawrence Livermore National Laboratory, SIMON MACLEOD, Atomic Weapons Establishment, MAGNUS J. LIPP, ZSOLT JENEI, J.H. PARK KLEPEIS, Lawrence Livermore National Laboratory, YUE MENG, STANISLAV SINOGEIKIN, HP-CAT, APS — Naturally oxidized uranium has been compressed using a diamond anvil cell. Although X-ray diffraction shows the anisotropic nature in the pressure dependent changes to the lattice parameters of pure uranium as previously recorded, uranium oxide appears stable at high pressure in the fcc phase without clear evidence of a phase transition. The lattice parameters of uranium oxide formed by natural surface oxidation have been determined along with those of the underlying pure uranium employing Rietveld refinement. We will discuss the seemingly unexpected findings about uranium oxide.

1Work performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344. Diffraction studies were performed at HPCAT (Sector 16), APS/ANL. HPCAT is supported by CIW, CDAC, UNLV and LLNL through funding from DOE-NNSA, DOE-BES and NSF. APS

3:54PM L31.00008 Uranium hydride (UH\textsubscript{3}) and deuteride (UD\textsubscript{3}) under conditions of high pressure and temperature, MAGNUS LIPP, ZSOLT JENEI, JAE HYUN PARK KLEPEIS, BRUCE BAER, HYUNCHAE CYNN, WILLIAM EVANS, DON FUJINO, Lawrence Livermore National Laboratory, BLAKE NOLAN, JOE WERMER, Los Alamos National Laboratory, CHANGYONG PARK, DMITRY POPOV, HP-CAT, Advanced Photon Source, Argonne National Laboratory — Uranium hydrides are currently being evaluated as fuels for extreme conditions. They also serve as sources for very clean hydrogen by decomposing when heated at ambient pressure. We have examined their behavior over a large pressure and temperature range by placing small quantities and a pressure marker in a diamond anvil cell for angle dispersive x-ray diffraction. Neutron was chosen as pressure transmitting medium to ensure the best possible hydrostatic conditions. We'll discuss crystal structures, the equation of state, the bulk modulus and the phase diagram. Work performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344. Diffraction studies were performed at HPCAT (Sector 16), APS/ANL. HPCAT is supported by CIW, CDAC, UNLV and LLNL through funding from DOE-NNSA, DOE-BES and NSF. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH11357.

4:06PM L31.00009 Structural Stabilities and Electronic Properties of Cobalt Hydrides, YASUYUKI MATSUIURA, TATSUYA SHISHIDOU, ADSM, Hiroshima University, TAMIO OGUCHI, ISIR, Osaka University, ADSM, Hiroshima University — Cobalt forms ferromagnetic hydrides CoH\textsubscript{x}, at high pressures of hydrogen [1]. As the hydrogen pressure increases at temperatures 250-350°C, the concentration of hydrogen in the hcp phase monotonically increases, and reaches \( x \sim 0.6 \) at 7 GPa. At higher pressures, an fcc-based hydride with \( x \sim 1.0 \) is formed. At ambient pressure and 120 K, hydrogen atoms in the solution with \( x \leq 0.26 \) are randomly distributed over octahedral interstitial sites [2]. In the solution with \( x = 0.34 \) (\( x \geq 0.35 \)), hydrogen atoms occupy every third (second) layer. The magnetic moments of the hcp-based hydrides are oriented to the c-axis, and are decreased with increasing hydrogen concentration at a rate of about 0.36 \( \mu_B \) per hydrogen atom. In this study, we optimize the structural parameters for several structures, and investigate the structural stabilities and related electronic properties by using first-principles calculations. The full-potential linearized augmented plane wave method with the generalized gradient approximation is adopted.


4:18PM L31.00010 Formation of collapsed tetragonal phase in EuCo\textsubscript{2}As\textsubscript{2} under high pressure, MATTHEW BISHOP, University of West Georgia (UWG), Carrollton, GA 30018, USA, WALTER UHOYA, GEORGIY TSOI, YOGESH VOHRA, University of Alabama at Birmingham (UAB), Birmingham, AL 35294, USA, ATHENA SFEAT, BRIAN SALES, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN 37831, USA — The structural properties of EuCo\textsubscript{2}As\textsubscript{2} have been studied up to 35 GPa, through the use of x-ray diffraction in a diamond anvil cell at a synchrotron source. At ambient conditions, EuCo\textsubscript{2}As\textsubscript{2} (\textit{I}4/mmm) has a tetragonal lattice structure with a bulk modulus of \( 48 \pm 4 \) GPa. With the application of pressure, the \( a \) axis exhibits negative compressibility with a concurrent sharp decrease in \( c \) axis length. The anomalous compressibility of the \( a \) axis continues until 4.7 GPa, at which point the structure undergoes a second-order phase transition to a collapsed tetragonal (CT) state with a bulk modulus of 111 \pm 2 GPa. We found a strong correlation between the ambient pressure volume of 122 parents of superconductors and the corresponding tetragonal to collapsed tetragonal phase transition pressures.

3MB acknowledges support from the National Science Foundation (NSF) Research Experiences for Undergraduates (REU)-site under grant no. NSF-DMR-06146842.

4:30PM L31.00011 The behavior of semi-metal Bi\textsubscript{1}Te\textsubscript{3} under pressure, JASON JEFFRIES, Lawrence Livermore National Laboratory, A. L. LIMA SHARMA, Sandia National Laboratory and San Jose State University, P.A. SHARMA, C. D. SPATARU, Sandia National Laboratory, S.K. MCCALL, Lawrence Livermore National Laboratory, J.D. SUGAR, Sandia National Laboratory, S.T. WEIR, Lawrence Livermore National Laboratory, Y. K. VOHRA, University of Alabama, Birmingham — As a member of the \( (\text{Bi}_2)_m \text{Bi}_n \text{Te}_3 \) adaptive series, \( \text{Bi}_1\text{Te}_3 \) exhibits identical crystallographic symmetry and similar electronic properties to the archetypal thermoelectric material \( \text{Bi}_2\text{Te}_3 \). The extra Bi atoms in \( \text{Bi}_1\text{Te}_3 \) serve to increase the electronic density of states, making \( \text{Bi}_1\text{Te}_3 \) a semi-metal, as opposed to semiconducting \( \text{Bi}_2\text{Te}_3 \), at ambient pressure. We will report the results of high-pressure structural and magnetotransport characterization of \( \text{Bi}_1\text{Te}_3 \), focusing on the interplay between structural parameters and the underlying electronic properties. Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344.

4:42PM L31.00012 Theoretical X-ray Spectroscopy for Strongly Correlated Materials at High Pressure, ADAM P. SORINI, CHENG-CHIEN CHEN, SHIBING WANG, WENDY L. MAO, THOMAS P. DEVEREAUX, Stanford Institute for Materials and Energy Science, CHI-CHANG KAO, SSRL, SLAC National Accelerator Laboratory — We present theoretical x-ray spectra for correlated d- and f-electron materials under extreme conditions. We use exact-diagonalization to study small clusters of atoms including ligand charge-transfer and atomic-multiplet effects. These techniques allow us to extract information from spectroscopic measurements regarding phase transitions in strongly correlated materials as a function of pressure. We show recent results for hematite (Fe\textsubscript{2}O\textsubscript{3}) which undergoes a variety of phase transitions (structural, spin, metal/insulator) near 50 GPa, which have been observed using hard x-ray quadrupolar absorption. We also apply our models to the correlated f-electron “volume collapse” systems which show complex behavior under pressure.

1DOE Grant No. DE-AC02-76SF00515 and No. DE-FG02-08ER46540
4:54PM L31.00013 Fermi surface of SnO under pressure, NIELS CHRISTENSEN, AXEL SVANE, Aarhus University — Tin monoxide undergoes a pressure induced insulator-metal transition around 5 GPa. The pressure effects on the electronic band structure, the Fermi surface (FS) and its nesting properties of SnO in the metallic phase have been derived from ab initio calculations within the local density (LDA) and quasiparticle selfconsistent GW (QSGW) approximations. It is found that the topologies of the FS determined by the two approaches are very similar. Nesting occurs between two different sheets of the FS, most pronounced via (1,1,0) Q-vectors connecting the outer electron surface with the hole surface. The present study was motivated by recent observation of superconductivity in SnO under pressure [1].


5:06PM L31.00014 Dynamic response of Cu46Zr54 metallic glass to high-strain-rate shock loading: Plasticity, spall, and atomic-level structures, BEDRI ARMAN, Texas A&M, SHENG-NIAN LUO, TIMOTHY GERMANN, Los Alamos National Laboratory, TAHIR CARGIN, Texas A&M — Dynamic response of Cu46Zr54 metallic glass under adiabatic planar shock wave loading with molecular dynamics simulations was investigated. We analyzed the Hugoniot (shock) states up to 60 GPa, shock-induced plasticity and dynamic spall strengths. Especially, the spall strengths likely represent the limiting values achievable in experiments such as laser ablation. To characterize local deformation and structure at various stages of shock, release, tension and spallation, the local von Mises shear strain and Voronoi tessellation analyses were used. Modeled glass showed plasticity as localized shear transformation zones rather than thermal origin. Nucleation of voids occurred preferentially at the highly shear-deformed regions. Our simulations through the Voronoi and shear strain analyses suggest that the atoms having different local structures are of different shear resistances that lead to shear localization.

5:18PM L31.00015 Single Crystal X-ray Diffraction at Megabar Pressures and Temperatures of Thousands Degrees, LEONID DUBROVINSKY, NATALIA DUBROVINSKAIA, MARCO MERLINI, MICHAEL HANFLAND — The most reliable information about crystal structures and their response to changes in pressure and temperature is obtained from single crystal diffraction experiments. We have developed a methodology to perform single crystal X-ray diffraction experiments in laser-heated diamond anvil cells and demonstrate that structural refinements and accurate measurements of the thermal equation of state of metals, oxides, silicates from single crystal intensity data is possible in a pressures ranging up to megabars and temperatures of thousands degrees. New methodology was applied to solve in situ high-pressure high-temperature structure of iron oxide and study structural variations of iron and aluminum bearing silicate perovskite at conditions of the Earth lower mantle.

Wednesday, March 23, 2011 8:00AM - 11:00AM — Session P31 DMP GSCCM DCOMP: Focus Session: Materials at High Pressure IV: Geophysical Materials and Magnetic Transitions C145

8:00AM P31.00001 Pressure-induced phase transitions in NaMgF3 post-perovskite1, KOICHIRO UMEMOTO, Department of Geophysics and Geology, University of Minnesota, RENATA WENTZCOVITCH, MSI and CEMS, University of Minnesota — Understanding the behavior of MgSiO3 post-perovskite (PPV) under extreme pressures is fundamental for modeling the interiors of solar giants and extrasolar planets. In 2006, MgSiO3 post-perovskite was predicted to dissociate into MgO and SiO2 at 1.1 TPa (Umemoto et al., Science 311, 983 (2006)). However, the predicted dissociation pressure is too high to be easily verified experimentally. Instead, a low-pressure analog, NaMgF3 neighborite, has been studied to test for structural predictions in MgSiO3. NaMgF3 was predicted to dissociate at ~40 GPa (Umemoto et al., Geophys. Res. Lett. 33, L15304 (2006)), but this has not been confirmed experimentally (Martin et al., Geophys. Res. Lett. 33, L11305 (2006); Grocholski et al. Geophys. Res. Lett. 37, L14204 (2010)) and the dissociation MgSiO3 PPV is now being questioned. Here, we reexamine in detail the pressure dependence of crystal structures and phonon frequencies in NaMgF3 and reveal the apparent reason why dissociation was not observed in this material.

1Work supported by NSF under ATM-0428774 (VLab), EAR-0757903, and EAR-1019853. Computations were performed at MSI and Laboratory for Computational Science and Engineering (LCSE).

8:12AM P31.00002 First-principles calculation of thermal conductivity of silicate perovskite at high pressures and high temperatures, JIANJUN DONG, Auburn University, XIAOLI TANG, California Institute of Technology, ABBY KAVNER, UCLA, MOSES NTAM, Auburn University — The lattice thermal conductivity of silicate perovskite, the most abundant mineral in the Earth’s lower mantle, is calculated by combining the first-principles electronic structure theory and Peierls-Boltzmann transport theory. The phonon scattering rate due to lattice anharmonicity and Mg/Fe mass disorder is evaluated for each mode at the extreme P-T conditions of the lower mantle. The predicted thermal conductivity of single crystal MgSiO3 perovskite at ambient condition, about 5.7 W/m/K, is in excellent agreement with experiment. Adding about 0% Fe will lower the thermal conductivity by nearly 40%. Our calculation also reveals an unique pressure dependence for the thermal conductivity of perovskite, and the calculated thermal conductivity of iron bearing perovskite is almost an order of magnitude lower than the previously estimated based on long extrapolation of single crystal data. Including a re-evaluation of radiative contribution, we discuss the implications of our results for the heat flow in deep Earth.

2Funded by NSF (EAR-0757847)

8:24AM P31.00003 Identification of post-pyrite transition in SiO2 by a genetic algorithm, SHUNQING WU, Iowa state U and Xiamen U, KOICHIRO UMEMOTO, GEÔ, U of Minnesota, KAI-MING HO, MIN JI, CAI-ZHUANG WANG, Ames Lab, Iowa state U, RENATA WENTZCOVITCH, MSI and CEMS, U of Minnesota — Here we propose a new phase of SiO2 by a genetic algorithm showing that SiO2 should undergo a post-pyrite transition to a hexagonal phase, not to the cotunnite phase. The hexagonal phase is energetically very competitive with the cotunnite-type one.

1This work was supported by the U.S. Department of Energy, Office of Basic Energy Science, Division of Materials Sciences and Engineering and NSF under ATM-0428774 (VLab), EAR-0757903, and EAR-1019853.
8:36 AM P31.00004 Spin crossover systems in the deep mantle. RENATA WENTZCOVITCH, Department of Chemical Engineering and Materials Science, Minnesota Supercomputing Institute, University of Minnesota — In recent years there has been much interest on spin crossovers found experimentally in the most abundant minerals of Earth’s lower mantle ((Mg,Fe)O and (Mg,Fe)(Si,Fe)O$_2$-perovskite) under pressure. Spin crossovers are strongly dependent on thermodynamic conditions and a full understanding of this problem requires its investigation as function of pressure and temperature. There are several controversies, especially in the perovskite systems, and surprises are revealed by electronic structure calculations. The geophysical consequences of these crossovers are yet to be fully understood but could be fascinating. I will review progress we have made in understanding spin crossovers and give an overview of this phenomenon and its potential implications for the Earth.

Research carried out in collaboration with H. Hsu, K. Umemoto, P. Blaha, J. F. Justo, and C. R. S. da Silva. Research supported by the MRSEC Program of NSF under Award Number DMR-0212302 and DMR-0819885, and by NSF/ATM-0428774, EAR-0810212, and EAR-1047629.

9:12 AM P31.00005 Insulator to Metal and Magnetic Transitions in FeO under High Pressure: DFT-DMFT Computations. R. E. COHEN, Geophysical Laboratory, Carnegie Institution, KRISTJAN HAULE, GABI KOTLIAR, Rutgers University — We have applied DFT+Dynamical Mean Field Theory (DMFT) to FeO under varying pressure and strain to understand possible transitions in FeO. We use a LAPW basis set, and the lattice terms are evaluated using the WIEN2K LAPW code. The impurity model is solved using continuous time quantum Monte Carlo (CTQMC). Temperature enters explicitly, so we made special efforts to understand high temperature behavior relevant to geophysics. The computations are fully self-consistent, including the impurity levels and crystal field splitting, and the total energy is evaluated using the full potential and charge density of the lattice plus impurity models. We find with increasing pressure in paramagnetic FeO in a cubic lattice and $U=8$ eV a high-spin-low-spin transition, with a possible intermediate spin state (characterized by intermediate occupancies of the t2g and eg states) between. We find that at 300K cubic FeO remains insulating to a factor of two compression (over 600 GPa). However, high temperatures (e.g. 2000K) and rhombohedral lattice strain promote a metal insulator transition. We are delineating the phase boundaries. This work is supported by NSF.

9:24 AM P31.00006 First-principles study of spin-state crossovers and hyperfine interactions of ferric iron in magnesium silicate perovskite. HAN HSU, University of Minnesota, PETER BLAHA, TU Vienna, MATTEO COCCOCCI, RENATA WENTZCOVITCH, University of Minnesota — The spin-state crossover in iron-bearing MgSiO$_3$ perovskite, the most abundant mineral in the Earth, may significantly affect the properties of Earth’s lower mantle. However, details of this phenomenon have been very unclear, owing to the complicated nature of this mineral, mainly the coexistence of ferrous and ferric iron. Using the density functional theory plus Hubbard $U$ (DFT+U) methods, we investigated the spin states and hyperfine interactions of ferric iron in this mineral. We show that a crossover from high-spin to low-spin state occurs within the lower-mantle pressure range, and it is accompanied by a noticeable volume reduction and an increase in iron nuclear quadrupole splitting (QS). These results are consistent with recent x-ray diffraction and Mossbauer spectroscopy measurements [K. Catalli et al., Earth Planet. Sci. Lett. 289 (2010)].

This work is primarily supported by the MRSEC Program of NSF under DMR-0212302 and DMR-0819885, and partially supported by EAR-0810212 and EAR-1047629. P.B. was supported by the Austrian Science Fund (P20271-N17). Calculations were performed at MSI.

9:36 AM P31.00007 Ab initio melting curve of Fe and Fe-B alloys at extreme pressures: implications for Earth’s and exoplanet’s cores. JOHANN BOUCHET, CEA, GUILLAUME MORARD, Institut de Minéralogie et de Physique des Milieux Condensés, STEPHANE MAZEVET, CEA, FRANCOIS GUYOT, Institut de Minéralogie et de Physique des Milieux Condensés — Exoplanets with masses similar to that of Earth have recently been discovered in extrasolar systems [1]. A first order question for understanding their dynamics is to know whether they possess Earth-like liquid metallic cores. However, the iron melting curve is unknown at conditions corresponding to planets of several times the Earth’s mass (over 15 Mbar for planets with 10 times the Earth’s mass [2]). In the density-temperature region of the cores of those super-Earths, we calculate the iron melting curve using first principle molecular dynamics simulations based on density functional theory. We also propose an equation of state for iron in this pressure range. Finally we show the melting curve of Fe$_3$S and discuss the effects of the addition of sulfur to the melting curve of pure iron.


9:48 AM P31.00008 Elasticity of iron-bearing olivine polymorphs investigated by first principles MARIBEL NUÑEZ VALDEZ, School of Physics and Astronomy, University of Minnesota, YONGGANG YU, Dept. of Chemical Engineering and Material Sciences, University of Minnesota, RENATA WENTZCOVITCH, Dept. of Chemical Engineering and Material Sciences and Minnesota Supercomputing Institute, University of Minnesota — We calculate by first principles the effect of iron on the high pressure-temperature elasticity of olivine polytypes: $\alpha$-phase (olivine), $\beta$-phase (wadsleyite) and $\gamma$-phase (ringwoodite), the major constituents of the Earth’s upper mantle and transition zone (TZ). We combine the LDA, the quasiharmonic approximation, and a model vibrational density of states for the solid solution to calculate the full elastic tensor $\beta_{ij}$. We present results on the range of stability of pure methane and discuss how the quasiharmonic approximation with a model vibrational density of states for the solid solution to calculate the full elastic tensor $\beta_{ij}$ bulk (K) and shear ($G$) moduli of (Mg$_{87}$Fe$_{13}$)$_3$SiO$_3$. Comparison with experimental data at ambient conditions validates our results. In the pressure and temperature range of the upper mantle and TZ we study single crystal wave propagation anisotropy and polarization anisotropy in aggregates with preferred orientation.

Research supported by NSF EAR-1019853 and EAR-0810272. Computations were performed at the Minnesota Supercomputing Institute.

10:00 AM P31.00009 Polymerization of methane in the deep Earth. LEONARDO SPANU, Department of Chemistry UC Davis, DAVIDE DONADIO, MPI for Polymer Research; Department of Chemistry UC Davis, DETLEF HOHL, Shell Global Solutions Inc. Houston, TX, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, Livermore CA, GIULIA GALLI, Department of Chemistry and Department of Physics, UC Davis — Determining physical and chemical properties of carbon fluids at high pressure and temperature is a key step towards understanding carbon reservoirs and fluxes in the deep Earth. The stability of carbon-hydrogen systems at depth greater than few thousands meters is poorly understood and the abiotic hypothesis on the synthesis of higher hydrocarbons (HCs) in the Earth mantle remains controversial. We have used ab initio molecular dynamics simulations to investigate the formation of higher HCs from dissociation of pure methane, and of methane in contact with carbon surfaces and transition metals, in a range of pressure of $2 - 30$ GPa and temperature $T = 900 - 4,000$ K [1]. We present results on the range of stability of pure methane and discuss how the interaction with transition metals or carbon deposits (graphite and diamond) affects the formation of higher HCs.

[1] Leonardo Spanu, Davide Donadio, Detlef Hohl, Eric Schweger, Giulia Galli (submitted)

Work supported by a grant from Stichting Shell Research (SSR).

10:12 AM P31.00010 Solubility and erosion of icy cores in giant planets. HUGH WILSON, BURKHARD MILITZER, University of California Berkeley — The core-mantle boundary of a giant planet consists of an interface between dense rock/ice below and fluid hydrogen-helium above. Whether this phase boundary remains stable, however, or whether the core material is dissolved and redistributed throughout the interior, remains unknown, and has major consequences for planetary interior and formation models. In this work we use density functional theory molecular dynamics calculations to compute the free energy of solubility for the icy components of the core into fluid hydrogen, to investigate whether solubility is thermodynamically preferred at the extreme temperature and pressure conditions prevalent at the core-mantle boundaries of Jupiter and Saturn. The consequences for Jupiter and Saturn, as well as for giant exoplanets, will be discussed.
10:24AM P31.00011 Post-stishovite transition in ALOOH-incorporated SiO$_2$: A first principles study$^1$, KATSUYUKI KAWAMURA, Tokyo Institute of Technology, KOICHIRO UMEMOTO, RENATA WENTZCOVITCH, University of Minnesota, KEI HIROSE, Tokyo Institute of Technology — In 2007, Newfoundland et al. [Proc. Nat. Acad. Sci. 104, 13588 (2007)] showed that the incorporation of ALOOH into SiO$_2$ significantly reduces the transition pressure between stishovite and CaCl$_2$-type phases. In the present paper, we investigate theoretically the effect of hydrogen and aluminum on this transition. First-principles calculations show that aluminum has no effect on the transition pressure. However, hydrogen bonds play a crucial role, suggesting that a cooperative redistribution of hydrogens aids the post-stishovite transition. Large-scale molecular dynamics simulations using model potentials confirm this effect and reveal the nature of the hydrogen motion. This effect produces a strong temperature dependence on the transition pressure and should make the latter sensitive to hydrogen content in the material.

$^1$This work was supported by NSF under ATM-0428774 (VLab), EAR-0757903, and EAR-1019853. The computations were performed at the Minnesota Supercomputing Institute (MSI).

10:36AM P31.00012 Thermodynamic properties of MgSiO$_3$ majorite and phase transitions near 660-km depth in MgSiO$_3$ and Mg$_2$SiO$_4$: a first principles study$^1$, YONGGANG YU, Virginia Tech, RENATA WENTZCOVITCH, University of Minnesota, VICTOR VINOGRAD, U. Frankfurt, ROSS ANGEL, Virginia Tech — Thermodynamic properties of MgSiO$_3$ tetragonal majorite have been calculated at high $P-T$ within the quasiharmonic approximation based on DFT using both LDA and GGA. The LDA results compare exceptionally well with measured thermodynamic properties. A classical Monte Carlo simulation based on a cluster expansion method demonstrates that disorder between Mg and Si in the octahedral sites in majorite does not occur below 3600 K within 30 GPa. The calculated phase boundaries between majorite ($m_j$), perovskite ($pv$), and ilmenite (il) MgSiO$_3$ agree much better with experiments by using GGA than by LDA. The Clapeyron slopes (CS) predicted by GGA and LDA are close to each other: 0.9 ± 1.7 MPa/K for $m_{j-pv}$, 6.9 ± 7.9 MPa/K for $m_j-il$, and −4.2 ± 3 MPa/K for il-$pv$ transition. The triple point predicted by GGA is at 21.8 ± 1 GPa and 1840 ± 200 K which is ~400 K lower than most experiments. Our calculations also reveal that wadsleyite decomposes to an amorphous majorite plus periclase above 2280 K with a large negative CS (−22 ± 12 MPa/K) and that ringwoodite decomposes to ilmenite plus periclase below 1400 K (1.2 MPa/K). The geophysical implications to mantle convection and the composition of the Earth’s transition zone will also be discussed.

$^1$NSF: EAR-0738692, EAR-1047629, and ATM-0082774 (VLab)

10:48AM P31.00013 A first-principles investigation of hydrous defect and IR frequencies in forsterite: The case for Si vacancies$^1$, MARC HIRSCHMANN, KOICHIRO UMEMOTO, RENATA WENTZCOVITCH, DAVID KOHLSTEDT, ANTHONY WITHERS, University of Minnesota — We investigate charge-balanced hydrous magnesium and silicon defects ([2H]$^3$Mg, [4H]$^3$Si) by first principles. Here we propose two lowest-energy hydrogen configurations for [4H]$^3$Si. With these new configurations, the distribution of OH-stretching phonon frequencies in Group I (> 3450 cm$^{-1}$) are better reproduced. Substitution of silicon with 4 hydrogens gives rise to significant elongation of distances between oxygen ions at the tetrahedron of the silicon vacancy. Our calculations indicate that the correlation between O-O distances and O-H-stretching phonon frequencies, which has been well established for hydrous minerals, does not apply directly to nominally anhydrous minerals and should not be used to determine the identity of the hydrous defects responsible for infrared absorption peaks.

$^1$This work was supported by NSF under EAR-0757903 and EAR-1019853. The computations were performed at the Minnesota Supercomputing Institute (MSI).


11:15AM Q31.00001 Crystal structure prediction using evolutionary algorithms: how to predict large and complex systems, ANDRIY LYAKHOV, Stony Brook University — Evolutionary crystal structure prediction proved to be a powerful approach in discovering new materials. Algorithm USPEX allows one to predict the most stable crystal structure for a given compound without requiring any experimental input. However, certain limitations are encountered for systems with a large number of degrees of freedom and complex energy landscapes. We explore the nature of these limitations and address them with a number of newly developed tools. For large systems a major problem is the lack of diversity. It is countered with modified variation operators that favor atoms with higher local order and a special initialization procedure for the first generation. For complex energy landscapes, the key problem is the possible existence of several energy funnels. To address this problem, we develop an algorithm incorporating the ideas of abstract “distance” between structures using the so-called "fingerprint function." We will compare the efficiency of the old and new algorithm USPEX for different systems and show that the range of application for algorithm is increased. Some systems, where old algorithm couldn’t find a solution are now solvable with the new algorithm. And the speed of finding the solutions for systems with the complicated energy landscape is substantially increased.

11:51AM Q31.00002 Prediction of complex high-pressure M-B crystal structures with an evolutionary algorithm, ALEKSEY KOLMOGOROV, SHEENA SHAH, ROXANA MARGINE, University of Oxford — We have carried out an ab initio ground state search in two binary metal-boron systems using an evolutionary algorithm [1] and identified remarkably complex configurations stabilized at high pressures [2,3]. An alkali-earth metal boride is shown to undergo a structural transformation from a semiconducting to a metallic state while a new semiconducting transition metal boride is stabilized at a composition known to have only metallic ground states. For the proposed candidate materials we calculate the electron-phonon coupling and demonstrate their potential to be phonon-mediated superconductors.

12:03PM Q31.00003 Structure prediction for molecular crystals using evolutionary algorithms: methodology and applications. QIANG ZHU, Geosciences Department, Stony Brook University — Evolutionary crystal structure prediction proved to be a powerful approach in determining the atomic crystal structure of materials. Here, we present a specifically designed algorithm for the prediction of the structure of molecular crystals. The main feature of this new approach is that each molecule is treated as a whole body, which drastically reduces the search space and improves the efficiency, but necessitates the introduction of new variation operators described here. We illustrate the efficiency of this approach by a search for ice (H2O) structures at zero pressure and temperature, which easily finds the structures of ice Ih and Ic, as well as the thermodynamically stable at these conditions ice XI. We successfully apply this method to finding the hitherto unknown structures of plastic phases of methane at high pressure. These structures are distinguished by an icosahedral packing of the molecules, and are likely candidate solutions for methane A and B.

1The author thanks Intel Corporation, Research Foundation of Stony Brook University, Rosnauka (Russia,contract 02.740.11.5102), and DARPA (grant 54751) for funding.

12:15PM Q31.00004 Burnett-Cattaneo Continuum Theory for Shock Waves. B.L. HOLIAN, Los Alamos National Laboratory, M. MARESCHAL, Université Libre de Bruxelles, R. RAVELO, University of Texas-El Paso — We model strong shockwave propagation, both in the ideal gas and in the dense Lennard-Jones fluid, using a refinement of earlier work [2] which accounts for the cold compression by a nonlinear, Burnett-like, strain-rate dependence of the thermal conductivity, and relaxation of temperature components on the hot, compressed side of the shock front. The relaxation of the disequilibrium among the three components of the kinetic temperature, namely, the difference between the temperature in the direction of a planar shock wave and those in the transverse directions, particularly in the region near the shock front, is accomplished by a rigorous application of the Cattaneo-Maxwell relaxation equation to a reference state, namely, the steady shockwave solution of linear Navier-Stokes-Fourier theory, along with the nonlinear Burnett heat-flux term. Our new continuum theory is in nearly quantitative agreement with non-equilibrium molecular-dynamics simulations under strong shockwave conditions.

1Part of this work supported by the U.S. Department of Energy under contract DE-AC5206NA25396.

12:27PM Q31.00005 High-pressure—high temperature studies of ammonia. JULIUS OJWANG, RYAN MCMILLIANS, ALEXANDER GONCHAROV, Carnegie Institution of Washington — Energetic materials are of great interest in energy and defense applications. We illustrate the efficiency of energetic materials with improved properties, such as reduced environmental impact, a crystalline solid Triaminoguanidinium 1-methyl-5-nitriminotetrazolate (TAG), C3H12N2O2, has recently been synthesized (Klápoté et al. 2008). We have studied the properties of TAG under static compression, and under reaction initiation at high pressure, using Raman and IR spectroscopy and x-ray diffraction. TAG appears to remain a stable, crystalline solid up to at least 35 GPa at room temperature. Laser initiation at 10-15 GPa reveals a rapid self-propagating reaction (deflagration) that consumes the sample, similar to other energetic materials such as nitromethane. Post-initiation products include crystalline molecular nitrogen (delta-phase), and nitrogen crystallites with regular defects. The formation of bulk molecular nitrogen during deflagration - in both phase segregated and impurity-hosting forms - distinguishes TAG from other known energetic materials, and suggests a pathway for the generation of novel phases from element-enriched energetic substances.

1This research was conducted under U.S. Army Research Office grant # 56122-CH-H.

12:39PM Q31.00006 High pressure—high temperature studies of ammonia. JULIUS OJWANG, RYAN MCMILLIANS, ALEXANDER GONCHAROV, Carnegie Institution of Washington — Raman scattering measurements and x-ray diffraction of ammonia have been made under simultaneous conditions of high temperature and high static pressure in the laser heated diamond anvil cell. The experimental results on phase transitions with pressure increase at room temperature are found to be in accord with previous studies [1]. Pressure was increased up to 52 GPa and temperature ramped up to 2000 K. On increasing temperature at high pressure, strong changes in the ammonia Raman spectra are observed, which could be associated with melting. On melting, ammonia undergoes partial decomposition into nitrogen and hydrogen. We also observed the appearance of new N-H stretch bands at high temperatures which may be related to the formation of new bonds. When quenched back to room temperature the starting phase of solid ammonia is recovered. The shift in frequencies of the vibron bands of nitrogen with pressure shows that it is phase segregated from ammonia.

12:51PM Q31.00007 Atomic structure and elastic properties at high pressure of aluminum oxynitride in cubic phase. I.G. BATYREV, J.W. MCCAULEY, B.M. RICE, G.A. GAZONAS, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD 21050, A.R. OGANOV, Department of Geosciences and Department of Physics and Astronomy, State University of New York, Stony Brook, NY 11794-2100 — The atomic structure and elastic properties of aluminum oxynitride spinel (AlON) at high pressure (up to 40 GPa) have been calculated from first principles. We have assumed an “ideal” stoichiometry of cubic AlON with 35.7 mole % AlN using the constant anion model. The elastic constants were calculated from independent strains that were applied to a unit cell, parameterizing the total energy as a function of the strain and from a stress-strain relationship. At ambient conditions a clustered distribution of N atoms has ~ 1 eV per 55 atoms higher total energy than for a random distribution and slightly, but systematically lower elastic constants. The pressure dependence of C_{11}, C_{12} and C_{44} for random and cluster distributions of N atoms was calculated in the range of 0-40 GPa by performing six finite distortions of the lattice and deriving the elastic constants from the strain-stress relationship. The calculated values of dC_{11}/dP are in the range of 4.0-6.2 and for dC_{44}/dP ∼=0.8-1.5. The estimates are in reasonable agreement with experimental measurements of polycrystalline AlON. The minimum energy structure of AlON was found using the evolutionary algorithm USPEX (Oganov & Glass, 2006).

1:03PM Q31.00008 In Situ Neutron and Synchrotron X-ray Diffraction Studies of Jarosite at High-Temperature High-Pressure Conditions. H. XU, Y. ZHAO, D. HICKMOTT, J. ZHANG, S. VOGEL, L. DAEMEN, M. HARTL, Los Alamos National Laboratory — Jarosite (KFe₃(SO₄)₂(OH)₆) occurs in acid mine drainage and epithermal environments and hot springs associated with volcanic activity. Jarosite is also of industrial interest as an iron-impurity extractor from zinc sulfide ores. In 2004, jarosite was detected by the Mars Exploration Rover Mössbauer spectrometer, which has been interpreted as a strong evidence for the existence of water (and possibly life) on ancient Mars. This discovery has spurred considerable interests in stability and structural behavior of jarosite and related phases at various temperature, pressure, and aqueous conditions. In this work, we have investigated the crystal structure and phase stability of jarosite at temperatures up to 900 K and/or pressures up to 9 GPa using in situ neutron and synchrotron X-ray diffraction. To avoid the large incoherent scattering of neutrons by hydrogen, a deuterated sample was synthesized and characterized. Rietveld analysis of the obtained diffraction data allowed determination of unit-cell parameters, atomic positions and atomic displacement parameters as a function of temperature and pressure. In addition, the coefficients of thermal expansion, bulk moduli and pressure-temperature stability regions of jarosite were determined.
1:15PM Q31.00009 Testing the minimum thermal conductivity model for amorphous polymers using high pressure. WEN-PIN HSIEH, Department of Physics, University of Illinois, Urbana, MARK LOSEGO, PAUL BRAUN, Department of Materials Science and Engineering, University of Illinois, Urbana, SERGEI SHENOGIN, PAWEL KEBLINSKI, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY, DAVID CAHILL, Department of Materials Science and Engineering, University of Illinois, Urbana — Pressure dependence of thermal conductivity provides a critical test of the validity of the model of the minimum thermal conductivity for describing heat transport by molecular vibrations of an amorphous polymer. We measure the pressure dependence of the thermal conductivity of poly(methyl methacrylate) (PMMA) brushes grafted from SiC substrates using a combination of time-domain thermoreflectance and SiC anvil cell techniques. We also determine the pressure dependence of the thermal conductivity from a computational model of amorphous polystyrene. In both cases, thermal conductivity as a function of pressure is accurately predicted by the minimum thermal conductivity model via the pressure dependence of the elastic constants and density.

1:27PM Q31.00010 The Influence of Crystal Structure on the Thermal Expansion Behavior of GeZnO4. MICHAEL CRAWFORD, R.L. HARLOW, W.E. GUISE, DuPont Company, R.A. FISHER, Los Alamos National Laboratory, W. WOERNER, J.B. PARISE, Stony Brook University, Q. HUANG, J.W. LYNN, NIST Center for Neutron Research, R. STEVENS, California Institute of Technology, B. WOODFIELD, J. BOERIO-GOATES, Brigham Young University, J. LASHLEY, Los Alamos National Laboratory, O. GOURDON, A. HUQ, Spallation Neutron Source, Oak Ridge National Laboratory, J. HORMADALY, Ben Gurion University, P.L. LEE, Y. ZHANG, Argonne National Laboratory — GeZnO4 synthesized at ambient pressure adopts the rhombohedral phenacite crystal structure, whereas cubic or tetragonal inverse spinel phases are formed at high pressures. We have measured the thermal expansion for all three forms of GeZnO4 at temperatures from 10 K to 400 K (or higher) using synchrotron x-ray powder diffraction. The phenacite form exhibits negative thermal expansion below 300 K, changing to positive thermal expansion above that temperature. In contrast to this behavior, the cubic and tetragonal inverse spinel phases exhibit positive thermal expansion below room temperature. Characterization of these materials using x-ray and neutron diffraction, as well as heat capacity and Raman spectroscopy, will be described. Possible structural reasons for the different thermal expansion behaviors of the phenacite and spinel forms of GeZnO4 will be discussed.

1:39PM Q31.00011 First-principles calculation of Ca2RuO4 at high pressure. NOBUMI MIYAWAKI, TATSUYA SHISHIDOU, Hiroshima University, TAMIO OGUCHI, Osaka University — It has been observed that the layered perovskite antiferromagnetic insulator Ca2RuO4 reveals a phase transition into a ferromagnetic metal at 0.5 GPa [1]. This insulator-metal transition is accompanied by a structural change with tilt and rotation of RuO6 octahedron within the space group Pbca. Above about 9 GPa, another transition from the ferromagnetic to superconducting phase has been recently reported [2]. The transition includes a structure change from Pbca to Bbcm. In this study, a first-principles calculation is performed to study the electronic structure of Ca2RuO4, especially focusing on the changes of Ru 4d states, with pressure. As the pressure is increased, calculated ferromagnetic spin moment of Ru is gradually decreased in Pbca owing to the widening of Ru 4d band. It is interesting that a ferromagnetic solution still exists in Bbcm. Similar structural changes (the tilt and rotation of RuO6 octahedron) take place in Ca2−xSrRuO4, where orbital hybridization with spin-orbit coupling (SOC) is crucial [3]. We also investigated effects of SOC, with the result that those appear even in the electronic structure of Ca2RuO4. Calculation results optimizing the structure will be also discussed. [1] F. Nakamura, et al., Phys. Rev. B 65, 220402(R) (2002). [2] P. L. Alireza, et al.: J. Phys.: Condens. Matter 22, 052202 (2010). [3] T. Oguchi, J. Phys. Soc. Jpn. 78, 044702 (2009).

1:51PM Q31.00012 Effect of high pressure on transport and structural properties of topological insulator Bi2Se3. J.J. HAMLIN, Department of Physics, University of California San Diego, J.R. JEFFRIES, Lawrence Livermore National Laboratory, N.P. BUTCH, P. SYERS, Department of Physics, University of Maryland, D. A. ZOCCO, Department of Physics, University of California San Diego, S.T. WEIR, Lawrence Livermore National Laboratory, Y.K. VOHRA, Department of Physics, University of Alabama at Birmingham, J. PAGLIONE, Department of Physics, University of Maryland, M.B. MAPLE, Department of Physics, University of California San Diego — We report a series of electrical resistivity, magnetotransport, and x-ray diffraction measurements on the topological insulator Bi2Se3 under pressures as high as 34 GPa. The results demonstrate that applied pressure can be used to controllably tune the transport properties without chemical substitution.

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