**Diamond-Anvil Cell Infrared Facility at the National Synchrotron Light Source II**

2017 COMPRES Annual Report

November 2016 – October 2017

Prepared by Zhenxian Liu and Russell J. Hemley

The George Washington University

**Overview**

**F**rontier Synchrotron **I**nfrared **S**pectroscopy Beamline under Extreme Conditions (FIS), the successor of NSLS-U2A, will be the first synchrotron infrared (IR) beamline on the NSLS-II experimental floor and a new home for the high-pressure infrared user community. With over $2M allocated from the NSLS-II FY16 operational budget, the construction of the FIS/MET beamline cabins has been completed and the end station set-up is underway. The integrated optical facility for far-IR to UV absorption and reflectance spectroscopy with conventional sources, together with laser Raman and photoluminescence spectroscopy will be available to users for experiments starting in early January. Procurement of the dipole vacuum chamber for IR beam extraction has been executed and partial component delivery and installation is expected in December 2017. Final/complete installation will take place in April 2018 with subsequent science commissioning and operation for general users starting in summer 2018. FIS/MET will adapt one of the novel design features of NSLS II – the large-gap IR dipole – to provide unparalleled brightness and more than an order of magnitude greater flux compared to U2A throughout much of the IR spectrum. It will also have the improved far-IR capabilities that have made the high-pressure synchrotron IR program at NSLS unique. The source will also have exceptional stability, critical for spectroscopic studies under extreme conditions such as static and dynamic compression and variable temperatures. Full synchrotron IR capacity is expected in the middle of 2018 that will enable diffraction-limited performance in the entire IR spectral region. Overall, FIS is not only the successor to NSLS-U2A but also brings the dedicated facility to a new level for optical spectroscopic studies under extreme P-T conditions.

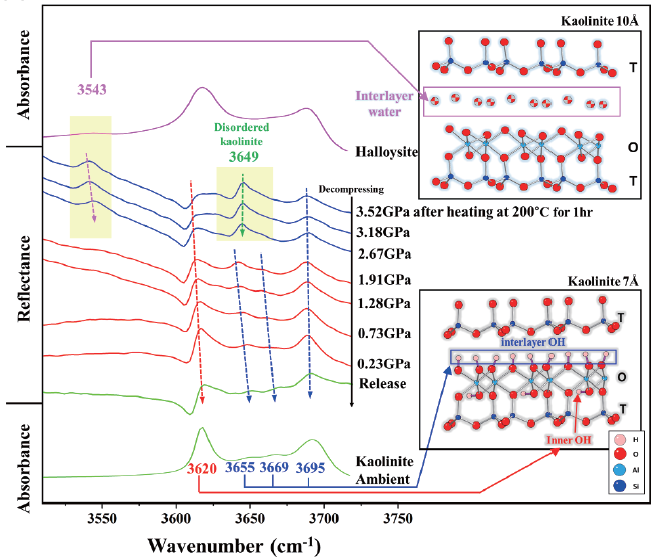
As a new and state-of-art integrated synchrotron IR facility, FIS will continue to be a COMPRES showcase for earth science and high-pressure research communities worldwide and a unique resource for the COMPRES user community. With the implementation of new developments/upgrades, the facility will allow for a wide range of micro-spectroscopic studies at broad range of pressures (over 300 GPa) and temperatures (from 5 Kelvin to several thousand K). Coupled with the synchrotron IR radiation, this facility will also provide diffraction-limited observation of diamond-cell samples in cryostats or under laser heated hot spots from the far to mid-IR spectral range. The new capabilities will greatly promote our users’ research projects to address problems ranging from outer solar system bodies to the Earth’s core, complemented by studies in materials science, condensed-matter physics, and chemistry (many of which are also carried out by the COMPRES user community).

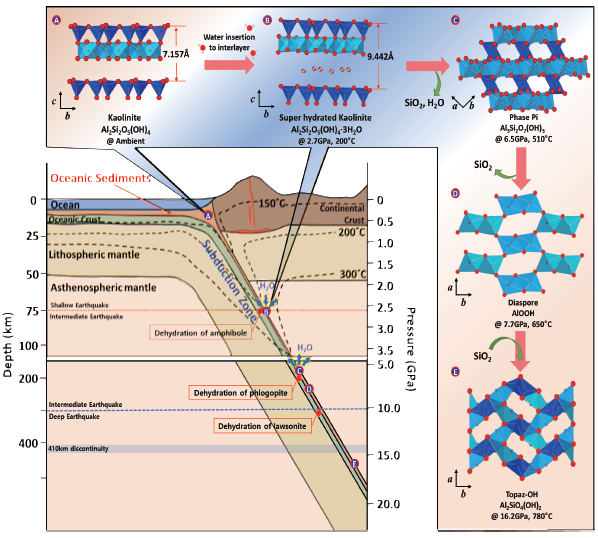
In addition, we established an offline infrared lab including FTIR and Raman spectroscopic systems, which have been made available to users since May 2016 (the first user research lab of NSLS-II accessible to general users) as well as the high-pressure IR program (Advanced Program) at the Advanced Light Source to bridge the gap/dark period between NSLS and NSLS-II. We also started to provide on-site and mail-in user support since January 2016.

**Scientific Highlights**

**a. *A role for Subducted Super-Hydrated Kaolinite in the Earth’s Deep Water Cycle***

Water is the most abundant volatile component in the Earth and influences both physical and chemical properties of the Earth materials. It continuously enters the Earth through subduction zones where it reduces the melting temperature of rocks to generate magmas while the rest travels further deep into the Earth. Our understanding of the water cycle in the Earth has emphasized dehydration processes along the subduction zones. A synergetic study led by Prof. Yongjae Lee from Yonsei University reveals that the formation and subsequent breakdown of super-hydrated kaolinite have important implications for water transport, volcanism, and possibly seismicity along the subduction zones. In-situ and time-resolved high pressure/high-temperature synchrotron X-ray diffraction and infrared spectroscopic techniques have been employed to characterize structural and chemical changes of kaolinite at conditions corresponding to those found in subduction zones. Synchrotron X-ray powder diffraction patterns of kaolinite at 2.7 GPa after heating to 200 °C in the presence of water, a condition corresponding to a depth of about 75km in cold slabs, show the appearance of a reflection with a d-spacing near 10Å which arises from pressure-induced insertion of water. IR reflectivity spectra measured following decompression from the super-hydrated kaolinite at 3.5 GPa after heating to 200 °C provide crucial evidence on hydration and dehydration, in excellent agreement with the XRD results. This new super-hydrated phase of kaolinite has a ~31 % larger unit cell volume and a ~ 8.4% lower density than the original kaolinite and has, with 29 weight-% H2O, the highest water content of any known aluminosilicate minerals in the Earth. As pressure and temperature approach 19 GPa and ca. 800 °C, the sequential breakdowns of super-hydrated kaolinite to phase-Pi, diaspore, and topaz-OH along with the formations of coesite and stishovite were observed. Breakdown of super-hydrated kaolinite in cold slabs subducted below 200 km then leads to the release of water that may further affect seismicity and help fuel arc volcanism at the surface.





***Figure 1.*** *Left: In-situ high-pressure IR reflectivity spectra of kaolinite during decompression from 3.5 GPa. For comparison, IR absorption spectra measured at ambient conditions of the original kaolinite and halloysite are shown as references on the bottom and top, respectively. The vertical dotted lines indicate the positions of the OH- stretching bands. Right: A schematic illustration of a (cold) subduction zone showing the super-hydration and breakdown sequence of kaolinite. Dehydration of amphiboles, phlogopite [K2(Mg,Fe)6Si6Al2O10·H2O] and lawsonite [CaAl2Si2O8·2H2O] are overlain for reference. Dashed black lines are the isotherms by Tsujimori, et al (Geol. S. Am. S.* ***403****, 147-168 (2006)).*

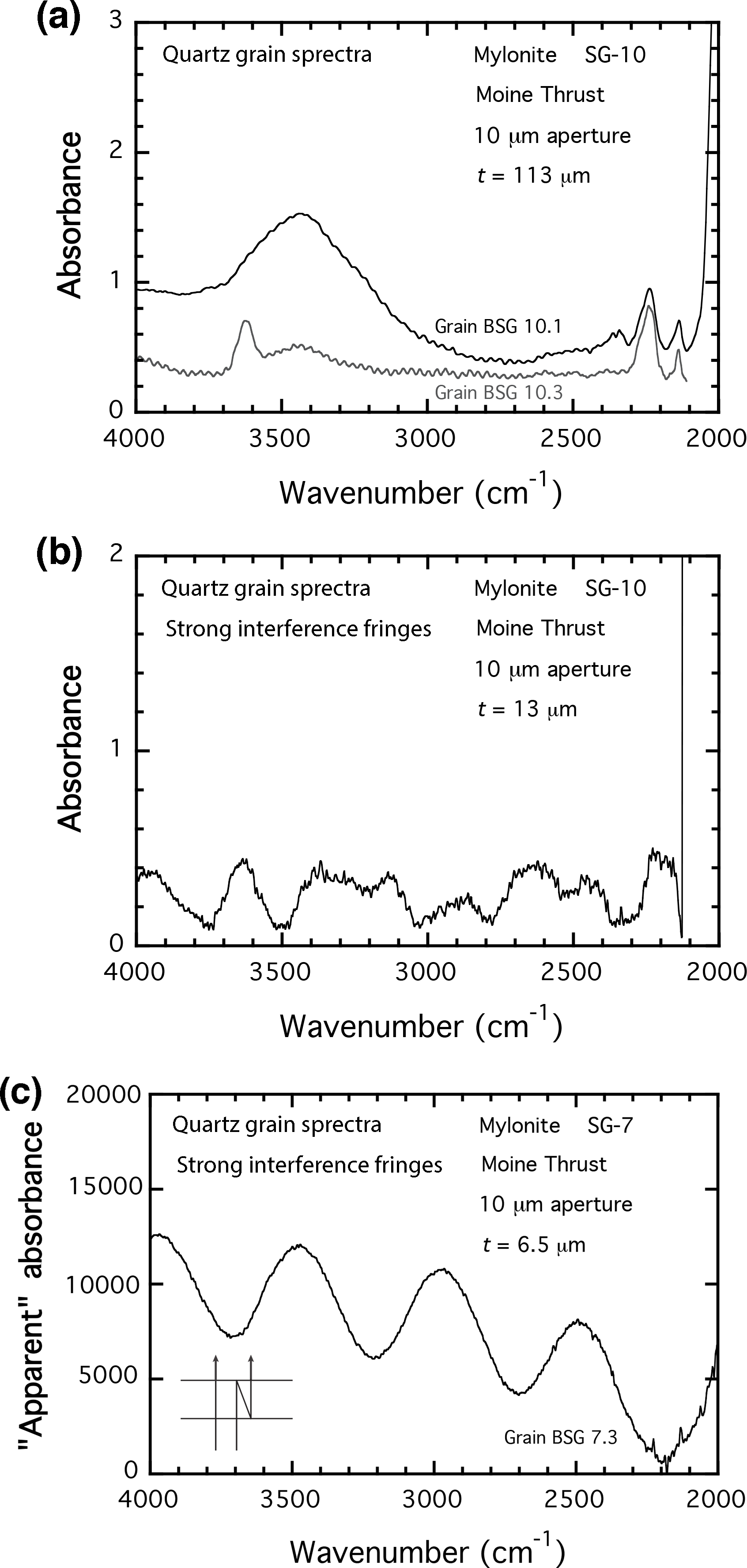
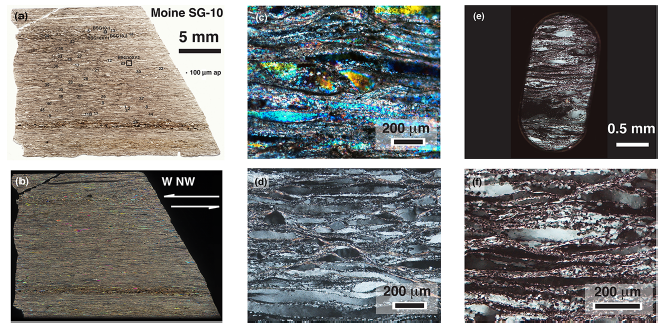
*Reference:* H. Hwang, D. Seoung, Y. Lee, Z. Liu, H. P. Liermann, H. Cynn, T. Vogt, C.C. Kao, and H.K. Mao, A Role for Subducted Siper-Hydrated Kaolinite in the Earth’s Deep Water Cycle, *Nature Geoscience*, in press.

***b. Synchrotron FTIR imaging of OH in quartz mylonites***

Previous measurements of water in deformed quartzites using conventional Fourier transform infrared spectroscopy (FTIR) instruments have shown that water contents of larger grains vary from one grain to another. However, the non-equilibrium variations in water content between neighboring grains and within quartz grains cannot be interrogated further without greater measurement resolution, nor can water contents be measured in finely recrystallized grains without including absorption bands due to fluid inclusions, films, and secondary minerals at grain boundaries. A team lead by Prof. Andreas Kronenberg of Texas A&M University utilized synchrotron infrared (IR) FTIR spectroscopic technique to distinguish and measure OH bands due to fluid inclusions, hydrogen point defects, and secondary hydrous mineral inclusions through an aperture of 10 μm for specimens > 40 μm thick. Doubly polished infrared (IR) plates can be prepared with thicknesses down to 4–8 μm, but measurement of small OH bands is currently limited by strong interference fringes for samples < 25 μm thick, precluding measurements of water within individual, finely recrystallized grains. By translating specimens under the 10 μm IR beam by steps of 10 to 50 μm, using a software-controlled x-y stage, spectra have been collected over specimen areas of nearly 4.5 mm2 . This technique allowed the team to separate and quantify broad OH bands due to fluid inclusions in quartz and OH bands due to micas and map their distributions in quartzites from the Moine Thrust (Scotland) and Main Central Thrust (Himalayas).

Mylonitic quartzites deformed under greenschist facies conditions in the footwall to the Moine Thrust (MT) exhibit a large and variable 3400 cm-1 OH absorption band due to molecular water, and maps of water content corresponding to fluid inclusions show that inclusion densities correlate with deformation and recrystallization microstructures. Quartz grains of mylonitic orthogneisses and paragneisses deformed under amphibolite conditions in the hanging wall to the Main Central Thrust (MCT) exhibit smaller broad OH bands, and spectra are dominated by sharp bands at 3595 to 3379 cm-1 due to hydrogen point defects that appear to have uniform, equilibrium concentrations in the driest samples. The broad OH band at 3400 cm-1 in these rocks is much less common. The variable water concentrations of MT quartzites and lack of detectable water in highly sheared MCT mylonites challenge our understanding of quartz rheology. However, where water absorption bands can be detected and compared with deformation microstructures, OH concentration maps provide insight into the histories of deformation and recovery, evidence for the introduction and loss of fluid inclusions, and water weakening processes.

*Reference:* A. Kronenberg, H. Hasnan, C. Holyoke III, R. Law, Z. Liu, J. Thomas, Synchrotron FTIR Imaging of OH in Quartz Mylonites, Solid Earth **8**, 1025–1045 (2017).

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***Figure 2.*** *Top: Doubly polished IR plates of Moine Thrust (MT) mylonites prepared perpendicular to foliation and parallel to lineation. (a) Lowmagnification image of large IR plate prepared from Stack of Glencoul sample SG-10 (unpolarized light), with a mean thickness t=120 μm. (b) Same IR plate of SG-10 shown in (a) but with crossed-polarized light. The MT top to WNW shear sense is shown in the plane of the IR plate (top to the left). (c) Higher magnification optical micrograph of large IR plate of sample SG-10, with crossed polarized light and local plate thickness (117 μm) determined from IR interference fringes. (d) Optical micrograph of Stack of Glencoul sample SG-7 in crossed-polarized light (normal 30 μm section thickness), illustrating deformation and recovery microstructures with higher resolution than in thick IR plates. (e) Low-magnification image of ultrathin IR plate of Stack of Glencoul sample SG-7-5 (crossed-polarized light) mounted on a copper TEM slot ring (t=4–8 μm, based on IR interference fringes). (f) Higher-magnification optical micrograph of the same IR plate SG-7-5 (crossed-polarized light) as shown in (e) with deformation and recrystallization microstructures shown more clearly than in normal 30 μm thin section.*

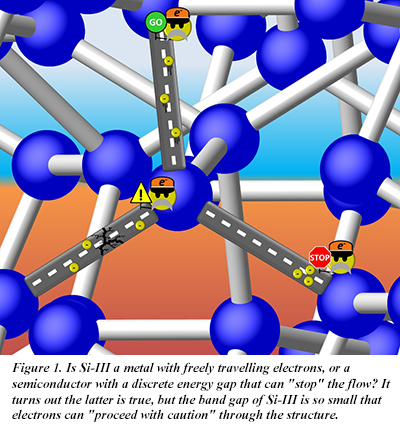
*Left: IR spectra of quartz grains in MT mylonite samples (Stack of Glencoul), measured with synchrotron–FTIR system using a 10 μm aperture with varying IR plate thicknesses (a) t=113 μm (BSG 10, local plate thickness determined from interference fringes), (b) t=13 μm (SG-10.2t), and (c) t=6.5 μm (BSG 7.3, sample plate SG-7-1). (a) IR spectra of MT sample (SG- 10) show OH absorption bands of similar character at the same wavenumbers for a 10 μm aperture as OH bands measured through a larger (100 μm) aperture, including a large broad absorption band at 3400 cm-1 due to dispersed fluid inclusions (both BSG 10.1 and BSG 10.3) and a sharper band at 3600 cm-1 due to mica inclusions (shown by BSG 10.3). Interference fringes in samples ~100 μm thick are apparent, allowing determination of local IR plate thickness, but they do not obscure the OH absorption bands. (b) Interference fringes for samples < 25 μm thick are large, and make detection of small OH absorption bands difficult. The only detectable absorbance bands in sample SG-10.2t (t=13 μm) are due to strong primary SiO vibrations (at υ < 2200 cm-1). (c) Interference fringes are very large for thin IR plates (t D6.5 μm; SG-7-1); neither SiO nor OH absorption bands are observed, even after attempts to model them and remove fringes numerically. All absorbance values (and apparent absorbance values of interference fringes exhibited by SG-7) are normalized to a uniform sample thickness of 1mm.*

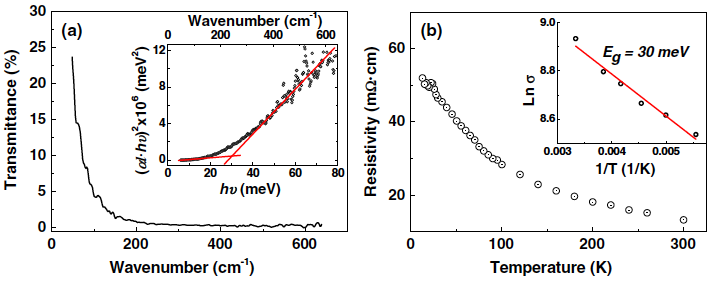
**c. *Direct Band Gap Silicon***

It is difficult to overestimate the importance of silicon when it comes to computing, solar energy, and other technological applications - not to mention the fact that it is the second-most abundant element in Earth’s crust, in terms of mass percent. The most common form of silicon crystallizes in the same structure as diamond (Si-I), but other allotropes can be created using different processing techniques. New work led by Tim Strobel at Geophysical Laboratory, Carnegie Institution of Washington shows that the Si-III (or BC8) phase, which is formed at high pressure, is a narrow band gap semiconductor.

The Si-I phase is a semiconductor and other known forms are metals, but the properties of Si-III have not been measured accurately until now. Previous experimental and theoretical research has suggested that Si-III is a poorly conducting metal, but due to the lack of sufficiently pure and sufficiently large crystals, the theoretical predictions have been difficult to verify experimentally.

​Lead scientist Haidong Zhang synthesized pure, bulk samples of Si-III synthesized with a large volume press technique, accurate measurements of the electronic properties of the material are now possible.  Key measurements of the far-IR spectrum performed at the Infrared Lab, NSLS-II by Zhenxian Liu show that Si-III is actually a semiconductor with a band gap of 30 meV. First-principles calculations reveal a direct band gap, in contrast to diamond-like silicon, which has an indirect band gap that is much larger, at 1.1 eV. This suggests that Si-III could have uses beyond the many applications in which diamond-like silicon is currently used.





***Figure 3.*** *Top:* (a) Optical transmittance spectrum for BC8-Si in the far-IR region. Tauc plot of the absorption, shown in the inset, reveals the fundamental direct band gap transition at ∼30 meV. (b) Temperature dependence of the electrical resistivity for BC8-Si. Inset shows the activation energy fit to the data between 300 and 180 K.

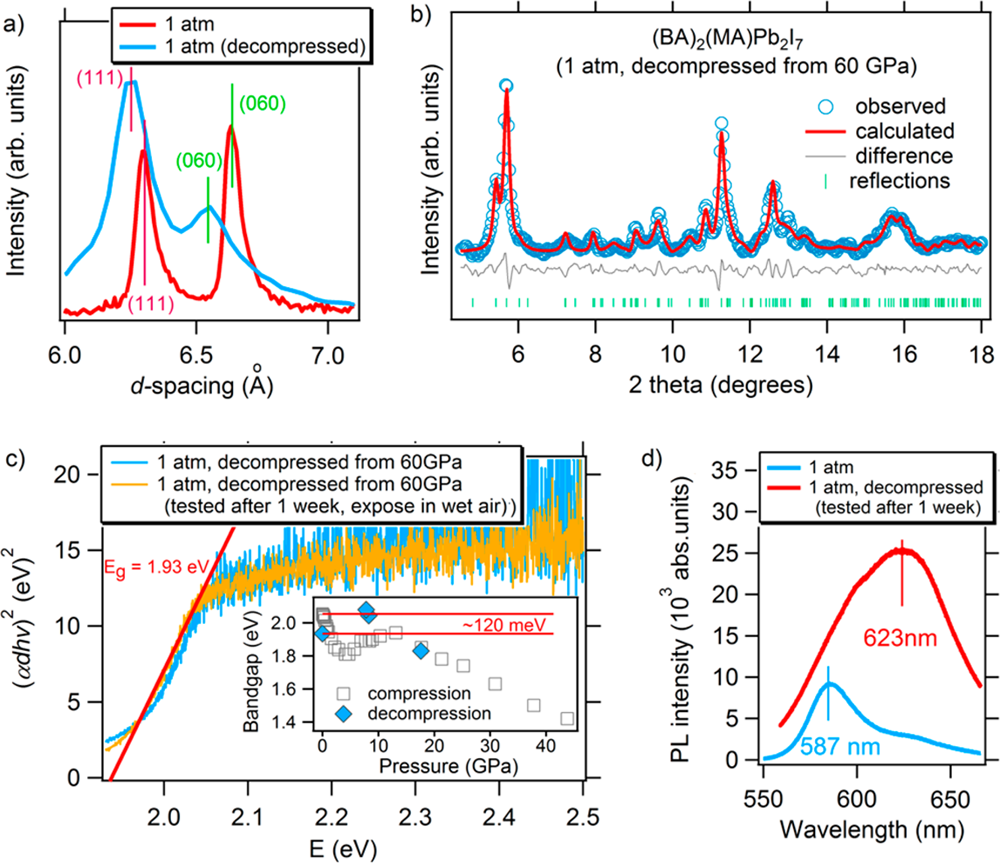
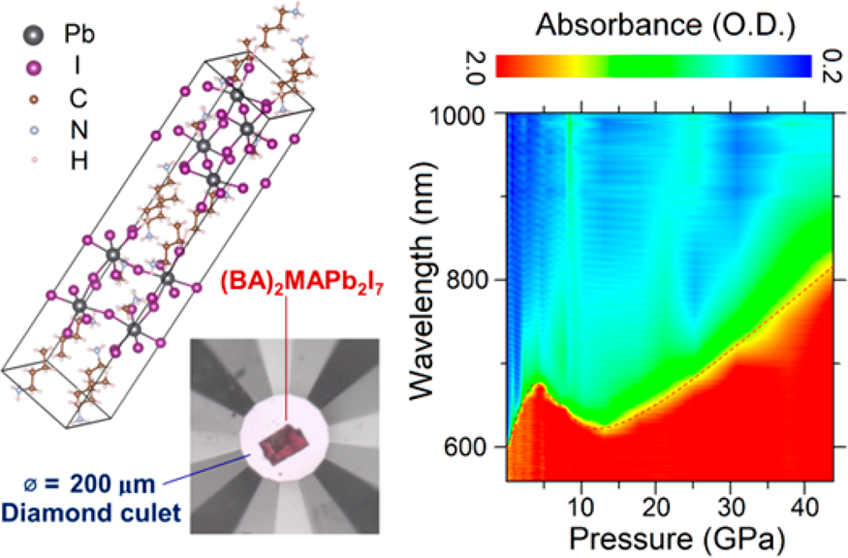
*Reference: H.* Zhang H. Liu, K. Wei, O. Kurakevych, Y. Godec, Z. Liu, G. Nolas, T. Strobel, BC8 Silicon (Si-III) is a narrow-gap semiconductor, *Phys. Rev. Lett*., **118**, 146601 (2017).

**d. *First High Pressure Study on 2D Hybrid Perovskites***

The power conversion efficiency of hybrid perovskites-based sola cell has been improved over 22%, whilst poor stability impedes its applications. This pushed researchers to investigate compositional and morphological variants. The recent developed two-dimensional layered perovskites show improved structure stability. However, the quantum confinement widens the band gap, which decreases the power conversion efficiency for low-cost, single junction devices. The discovery of elevated environmental stability in two-dimensional (2D) Ruddlesden−Popper hybrid perovskites represents a significant advance in low-cost, high-efficiency light absorbers. In comparison to 3D counterparts, 2D perovskites of organo-lead-halides exhibit wider, quantum-confined optical bandgaps that reduce the wavelength range of light absorption.

New work led by Dr. Gang Liu from HPSTAR characterized the structural and optical properties of 2D hybrid perovskites as a function of hydrostatic pressure and experimentally convinced a first example of pressure-improved 2D hybrid perovskites and proposed that pressure treatments might offer a useful route to yield near-ideal single junction performance in the 2D hybrid perovskites. Key measurements of the optical VIS-IR spectrum performed at the Infrared Lab, NSLS-II revealed that bandgap narrowing with pressure of 633 meV that is partially retained following pressure release due to an atomic reconfiguration mechanism. Two distinct regimes of compression dominated by the softer organic and less compressible inorganics sublattices are identified which never found in 3D hybrid perovskites. The research team also discovered two-step band-gap-redshift below 4 GPa and after 13 GPa from optical measurements. As both the two compressions will cause bandgap narrowing, the two-step bandgap shift can be attributed to the layer-to-layer and interlayer compressions, respectively

These findings, which also include PL enhancement, correlate well with density functional theory calculations and establish structure-property relationships at the atomic scale. These concepts can be expanded into other hybrid perovskites and suggest that pressure/strain processing could offer a new route to improved materials-by-design in applications.



***Figure 4.*** *Right: Ambient structure of 2D hybrid perovskites and their pressure-driven bandgap re-redshift behavior. Left: Retainable structural and electronic properties for (BA)2(MA)Pb2I7 decompressed from 60 GPa. (a) Noticeable change in relative intensities of (060) and (111) Bragg reflections between the as-prepared sample (before compression) and that decompressed from 60 GPa. (b) XRD pattern and GSAS refinement result of (BA)2(MA)Pb2I7. (c) Tauc plots for(BA)2(MA)Pb2I7 after compression. Bandgap magnitudes are stable after the sample is exposed to wet air for over 1 week. It can be clearly demonstrated that ∼120 meV bandgap narrowing has been achieved in the decompressed sample. (d) Comparison of PL spectra before compression and after decompression. A clear PL enhancement has been confirmed in the decompressed sample.*

*Reference:* G. Liu, L. Kong, P. Guo, C. Stoumpos, Q. Hu, Z. Liu, Z. Cai, D. Gosztola, H.K. Mao, M.G. Kanatzidis, and R.D. Schaller, Two Regimes of Bandgap Red Shift and Partial Ambient Retention in Pressure-Treated Two- Dimensional Perovskites, *ACS Energy Lett.*, **2**, 2518−2524 (2017).

**Beamline Personnel**

The management team is headed by PIs Russell J. Hemley (Professor, The George Washington University) and Zhenxian Liu (Research Associate Professor, The George Washington University). GWU serves as the funding host for the subaward of COMPRES-NSF Cooperative Agreement.

***Beamline Scientist***

Zhenxian Liu was appointed as a Research Scientist/Beamline Scientist at Carnegie since 2000. In July 2017, he was appointed as a Research Associate Professor at The George Washington University. He provided scientific and technical support to the high-pressure programs at the NSLS-U2A beamline over 15 years. He has a strong background in spectroscopy, solid-state physics, and multiple synchrotron techniques. He actively develops novel experimental techniques (e.g., vacuum far-IR spectroscopy down to 30 cm-1 at high pressure and cryogenic techniques with DACs down to 5 K and 360 GPa, far-IR reflectivity spectroscopy over megabar pressure, and off-line CO2 laser heating for DACs) and assists users in carrying out research projects in geoscience, planetary science, materials science, condensed matter physics, and chemistry. In addition, he uses synchrotron infrared spectroscopy, Raman scattering, photoluminescence as well as synchrotron x-ray diffraction techniques to explore physical and chemical properties and phase transitions of hydrous minerals, simple molecular systems, and nanoscale materials at high pressures and variable temperatures. During the transition period from NSLS to NSLS-II, his work and responsibilities include:

1. Coordinate with NSLS-II staff on beamline construction/developments at NSLS-II as the lead beamline scientist of FIS, the successor of NSLS-U2A. Current focus is the end station installation and technical developments as well as getting the Certificate of Beneficial Occupancy to allow the operating status to transition from the offline IR Lab to FIS beamline;
2. Manage and provide user support during the routine operation of the offline IR system at the Infrared Lab, NSLS-II. Current available GU time is equivalent to 50% of the NSLS-II beamline;
3. Provide on-site or remote support for high-pressure IR users at ALS beamline 1.4. Current beam time for high-pressure users is ~15-20% of that beamline.

***Junior Beamline Scientist***

Based on current schedule, the science commissioning will start in June following the beamline operation in the summer 2018. We request to increase the FIS operation funds to support a junior beamline scientist. This is critical to utilize FIS facility more efficiently and productively. A candidate search will begin as soon as the funds are committed.

**Beamline Operations**

Continuing effort has been made to keep operation of the IR Lab at NSLS-II and the high-pressure IR user program at ALS as routine. The IR Lab was officially open for general users in May 2016 as the first research laboratory available for general users through peer review process at NSLS-II. All user proposals have been reviewed and allocated laboratory time as General User Proposals (GUP). The custom IR microscope installed at ALS IR beamline 1.4 is available for all high-pressure IR users. That significantly increases the portion of beam time for high-pressure studies at 1.4 since we started our high-pressure IR program there to coordinate user beam time and provide on-site or remote user support. Special effort has been made to promote our users’ research projects on problems relating to high-pressure geoscience and planetary science, for instance, the investigation of subducted super-hydrated kaolinite for its role in the Earth’s deep water cycle. All these activities are summarized in Appendix 2 and 3. Our effort will continue to minimize the impact of the “dark period” due the NSLS shutdown and before the first IR light in June 2018 at FIS, NSLS-II.

**Beamline Developments:**

2017 was an exiting year for FIS beamline construction. More than $2M committed funds have be executed for two major procurements including the dipole vacuum chamber for IR beam extraction and acquisition/installation of the FIS/MET beamline cabins.

***a) FIS/MET cabin’s construction on the NSLS-II experimental floor and relocation and installation of FIS end stations***

The construction of the FIS/MET beamline cabins began in January 3, 2017 and completed in June 2017. Utility installations including nitrogen, helium, and argon gas supplies as well as compressed air and utility water have been completed in Novemebr. The relocation and installation of FIS end stations currently is under way. Two 4’ by 8’ optical tables has been installed (Figure 5) and three more will be installed shortly. The new FTIR spectrometer (Bruker Vertex 80) and another existing FTIR spectrometer (Bruker IFS 66v) have been installed. This allows us to simultaneously keep the IR Lab open for general users while relocating and installing rest of the equipment from the storage area. The two end stations will be ready for users in January 2018. All equipment from offline IR Lab is going to be moved and installed in FIS beamline at the end of 2017. All user experiments will be carried out in FIS cabins from January 2018.

**Planned Activities**

2018 will be a busy and exiting year for FIS beamline development as we are working on the end station installations and expecting to take the first synchrotron IR light in June following Science Commissioning and routine operation for general users in the summer. The planned activities include:

***a) End Station installation and beamline developments***

We will continue the FIS beamline end station installations to develop more capabilities for high-pressure user community. Once all the existing IR systems have been installed, major focus will be the development on external and internal heating DAC techniques. In collaboration with Dr. Bin Chen’s group of University Hawaii at Manoa, BX90 external heating DACs now are available for general users to carry out in-situ high P-T IR experiments with resistive heating. Ongoing development on in-situ laser heating DAC with synchrotron IR will become available for users as soon as a laser interlock system is installed at FIS front end station, the CO2 laser (currently in the storage area of NSLS-II but will be move into the FIS cabin in December) safety operation procedure (SOP) is approved, and the synchrotron IR beam comes online. These techniques will be greatly benefit the COMPRES user community and enable frontier research related to geosciences.

***b) Planned installation of dipole vacuum chamber for IR beam extraction***

The fabrication of the dipole vacuum chamber for IR beam extraction is currently under way. New upper half of dipole chamber fabrication was completed successfully. The installation of M1-M4 vacuum system will take place at the NSLS-II storage ring during the December 2017





*Figure 5. Relocation and installation of FIS end station is under way. Left: 4’× 8’ optical table and new FTIR spectrometer (Bruker Vertex 80) in the front end station (laser interlock to be installed); Right: 4’× 8’ optical table and Bruker IFS 66v FTIR spectrometer installed at the second end station (user laboratory with variety optical systems to be installed).*

winter shutdown period and dipole chamber will be installed in April following the Instrument Readiness Review (IRR) and first light in June. We will continue to actively engage in the process and ensure the feasibility for coupling the synchrotron IR beam with the two end stations inside the FIS cabin. We will start to set up the beam delivery pipe system in early 2018 following user’s science commissioning in June and routine operation for general users in the summer 2018.

***c) Planning FIS/MET “Kick-off” workshop during the NSLS-II User’s Meeting in May 21-23, 2018***

Given the fact that FIS together with MET (Magnetospectroscopy, Ellipsometry and Time-Resolved Optical Spectroscopies Beamline) as the first synchrotron IR facilities at NSLS-II will be ready for general users in summer 2018, we are planning to propose a combined FIS/MET workshop on “Synchrotron Infrared Spectroscopy on Materials in Extreme Environment”. This on-site workshop will bring together synchrotron-IR users to discuss the applications of the high-pressure IR spectroscopy in geoscience and planetary science as well as condensed matter physics and materials science. These techniques include the unique instrumentation at NSLS-II, such as high-pressure far-IR spectroscopy, coupling with Raman and other optical methods, and in vacuum or low/high temperature experiments, all of which will be available for general users. Also new developments in the field, including in-situ laser heating high P-T IR spectroscopy, synchrotron IR spectroscopy under high pressure and high magnetic field, and dynamic compression with synchrotron IR radiation will be discussed. A workshop proposal for COMPRES funding support will be submitted to the Education, Outreach and Infrastructure Development Committee shortly.

**Budget**

Actual and anticipated spending for beamline operations (May 2017– June 2018):

**1. Budget for Beamline Operations: June 2017-May 2018**

|  |  |  |  |
| --- | --- | --- | --- |
| Personal:  Beamline Scientist\* | Salary plus fringe benefits | $169,695 | This includes a normal raise and cost of living adjustment for the beamline scientist |
| Materials/Supplies  a.  b. | NSLS-II fees & stockroom  Diamond anvils and heating cell accessories | $12,043  $6,000 | Routine beamline expenses including office spaces, phone charges, and materials related to the FIS end stations development.  Type IIa anvils and parts for external heating DACs required for dedicated use for high P-T experiments at the facility |
| Travel | Travel for senior personnel | $6,000 | Travel between BNL and Washington and to attend annual COMPRES and other scientific meetings |
|  | Total direct cost | **$193,738** |  |
| **Total** |  | **$244,110** | This total includes indirect costs\*\* at a rate of 26% ($193,738×1.26). |

\* Fringe benefits: The GWU’s fringe benefit rate is 25.7%. Fringe benefits include normal costs associated with employment such as retirement, Social Security, Medicare, disability insurance, health insurance and other required taxes. Salaries are based on a full calendar year and include all leave taken.

\*\* Indirect costs: The off-campus indirect cost rate is 26.0% of total modified direct costs (TMDC). Total modified direct costs are calculated as total direct costs minus equipment, and participant support Costs.

**2. Budget Request for Beamline Operation: June 2018-May 2019**

|  |  |  |  |
| --- | --- | --- | --- |
| Personal:  Beamline Scientists\* | Salary plus fringe benefits | $258,188 | This includes a normal raise and cost of living adjustment for one senior and one junior beamline scientists |
| Materials/Supplies  a.  b. | NSLS-II fees & stockroom  Diamond anvils and heating cell accessories | $17,463  $12,000 | Routine beamline expenses including office spaces, phone charges, and materials such as liquid helium  Type IIa anvils and parts for external heating DACs required for dedicated use for high P-T experiments at the facility |
| Travel | Travel for senior personnel | $6,000 | Travel between BNL and Washington and to attend annual COMPRES and other scientific meetings |
|  | Total direct cost | **$293,651** |  |
| **Total** |  | **$370,000** | This total includes indirect costs\*\* at a rate of 26% ($293,651×1.26). |

\* Fringe benefits: The GWU’s fringe benefit rate is 25.7%. Fringe benefits include normal costs associated with employment such as retirement, Social Security, Medicare, disability insurance, health insurance and other required taxes. Salaries are based on a full calendar year and include all leave taken.

\*\* Indirect costs: The off-campus indirect cost rate is 26.0% of total modified direct costs (TMDC). Total modified direct costs are calculated as total direct costs minus equipment, and participant support Costs.

**Appendices**

**1. A publication list for 2016 and 2017:**

Arveson, S.M., B. Kiefer, J. Deng, Z. Liu and K.M. Lee, Thermally-Induced Coloration of KBr at High Pressures, to be published.

Ciezak-Jenkins, J., and T. Jenkins, Shear Induced Weakening of the Hydrogen Bonding Lattice of the Energetic material 5,5′-Hydrazinebistetrazole at High-pressure, *J. Mol. Struct.*, **1129**, 313-318 (2017).

Hong, F., B Yue, Z. Liu, B. Chen, and H. Mao, Pressure-driven Semiconductor-semiconductor Transition and its Structural Origin in Oxygen Vacancy Ordered SrCoO2.5, *Phys. Rev. B: Condens. Matter*, **95**(2), 024115 (2017).

Hong, F., B. Yue, N. Hirao, Z. Liu, B. Chen, Significant Improvement in in Mn2O3

Transition Metal Oxide Electrical Conductivity via High Pressure, *Sci. Rep*. **7**, 44078(2017)

Hong, F, B. Yue, X. Wang, Z. Cheng, Z. Wang, M. Kunz, Z. Liu, B. Chen, and H.K. Mao,Pressure and Structure Driven Topological Insulator-Metal Transition in 2D Bi2Se3 Nanoflakes, *Nature Materials*, submitted.

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**2. List of users & affiliations**

**a) Users who performed experiments at the IR Lab, NSLS-II since November 2016:**

Yale University: Kanani Lee, and Sarah M. Arveson;

University of Chicago: Elizabeth Thompson and Anne Davis;

University of Tennessee: Janice Musfeldt, Amanda Clune, Nathan Harms and Kennth O’Neal;

New Jersey Institute of Technology: Andrei Sirenko and Taras;

PennState: Xiang Li and Stephen Juhl

HPSTAR: Xingguo Hong, Yang Ding, Jianbo Zhang, Hongshan Deng, Haiyan Zheng, Yajie Wang, Peijie Zhang, Hengzhong Zhang, Feng Ke, Weixin Liu, Junxiu Liu, Zhiqiang Chen, Lingkong Zhang, Jinlong Zhu, Hongliang Dong,

**b) Mail-in users at the IR Lab, NSLS-II and on-site users supported at 1.4.3 beamline, ALS**

Yale University: Kanani Lee and Sarah M. Arveson;

Yonsei University: Yongjae Lee, Huijeong Hwang and Donghoon Seoung;

University of Chicago: Elizabeth Thompson;

Arizona State University: Dan Shim and Helene Piet;

University of California at Santa Crus: Earl O'Bannon;

HPSTAR: Hong Fang and Bingbing Yue;

Geophysical Laboratory: Qianqian Wang, Tim Strobel, Ajay Mishra, and Muhetaer Aihaiti;

University of Saskatchewan: John Tse;

**c) High-pressure IR beam time and experiments performed at ALS 1.4 beamline, ALS**

Sang-Heon Shim, Arizona State University, 11/10-12/2016; 05/18-20/2017; 09/15-16/2017

Quentin Williams, University of California, Santa Cruz, 11/21-23/2016; 04/04-07/17

Elizabeth Thompson, University of Chicago, 06/13-17/2017

Zhenxian Liu, Geophysical Lab, CIW, AP beam time (10%)

**3. General user proposals for the high-pressure research lab (IR Lab) received since May 1, 2017:**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| [**Proposal ID**](http://passadmin.bnl.gov/FeasibilityReview/GetResourceRequests?ResourceRequests-sort=Proposal_ID-asc) | [**Title**](http://passadmin.bnl.gov/FeasibilityReview/GetResourceRequests?ResourceRequests-sort=Proposal_Title-asc) | [**PI**](http://passadmin.bnl.gov/FeasibilityReview/GetResourceRequests?ResourceRequests-sort=PI_Last_Name-asc) | [**Cycle**](http://passadmin.bnl.gov/FeasibilityReview/GetResourceRequests?ResourceRequests-sort=Cycle-asc) | [**Status**](http://passadmin.bnl.gov/FeasibilityReview/GetResourceRequests?ResourceRequests-sort=Status-asc) |
| 301898 | Measuring temperature dependent-IR for probing layer-to-layer interactions in layered clay minerals | Hengzhong Zhang | 2018-1 | Allocation |
| 302420 | Investigate the band gap and IR vibration behavior of novel 2D perovskites under high pressure condition | Gang Liu | 2018-1 | PRP Review |
| 302599 | Chemical Reactions of Ammonium Bicarbonate at High Temperature and High Pressure | Hengzhong Zhang | 2018-1 | PRP Review |
| 302603 | High-pressure spectroscopic studies on antiperovskite Re-Gd2SnC | Jungseek Hwang | 2018-1 | PRP Review |
| 302636 | Low temperature Raman scattering and IR reflectivity in multiferroics | Taras Stanislavchuk | 2018-1 | PRP Review |
| 302681 | High-pressure transformations of silver(II) fluoride as viewed from IR spectroscopy | Viktor Struzhkin | 2018-1 | PRP Review |
| 301857 | How do local lattice distortions trigger magnetic crossovers in molecule-based magnets? | Janice Musfeldt | 2017-3 | Allocated Time |
| 301890 | Phase diagram of Nano-confined water under pressure | Zhiqiang Chen | 2017-3 | Allocated Time |
| 301246 | Wavelength-dependent absorption of pressure media and its influence on temperature determination in high-pressure experiments with laser-heated diamond-anvil cells | Jie Deng | 2017-3 | Allocated Time |
| 301935 | Exploring the essence of super stable silica coating DNA-gold nanoparticle superlattices by high pressure | Chunli Ma | 2017-3 | Allocated Time |
| 302203 | Infrared and Raman spectroscopic studies of network-forming glasses under Extreme Conditions | Xinguo Hong | 2017-3 | Allocated Time |
| 302248 | Low temperature Raman scattering and IR reflectivity in multiferroics | Taras Stanislavchuk | 2017-3 | Allocated Time |
| 301246 | Wavelength-dependent absorption of pressure media and its influence on temperature determination in high-pressure experiments with laser-heated diamond-anvil cells | Jie Deng | 2017-2 | Closed |
| 301717 | FTIR spectroscopic investigation of the effect of Al-substitution on high-pressure dense hydrous magnesium silicates (DHMSs) | Lily Thompson | 2017-2 | Closed |
| 301778 | In-situ infrared spectroscopic studies of hydroxyl in micas at high pressures | Anne Davis | 2017-2 | Closed |
| 301786 | Mapping the binding site of SW209415 (+) on 15-PGDH using a footprinting assay | Janna Kiselar | 2017-2 | Closed |
| 301833 | The pressure induced polymerization of acetylene under low temperature | Haiyan Zheng | 2017-2 | Closed |
| 301857 | How do local lattice distortions trigger magnetic crossovers in molecule-based magnets? | Janice Musfeldt | 2017-2 | Closed |
| 301045 | Infrared and Raman spectroscopic studies of GeO2 and SiO2 glasses under Extreme Conditions | Xinguo Hong | 2017-2 | Closed |
| 301139 | Low temperature Raman scattering in multiferroics | Andrei Sirenko | 2017-2 | Closed |
| 301890 | Phase diagram of Nano-confined water under pressure | Zhiqiang Chen | 2017-2 | Closed |
| 301898 | Measuring temperature dependent-IR for probing layer-to-layer interactions in layered clay minerals | Hengzhong Zhang | 2017-2 | Closed |
| 301901 | Raman spectroscopy of magnetic excitations and lattice dynamics in Sr2IrO4 and Sr3Ir2O7 Mott insulators under high pressure at low temperature | Sorub Jesu | 2017-2 | Closed |
| 301935 | Exploring the essence of super stable silica coating DNA-gold nanoparticle superlattices by high pressure | Chunli Ma | 2017-2 |